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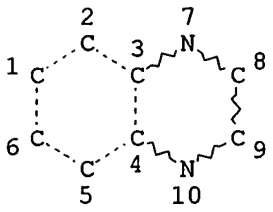
L1 STR

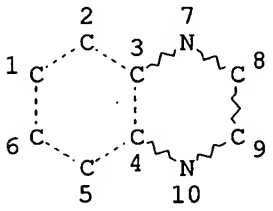


claim 27

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L3 52883 SEA FILE=REGISTRY SSS FUL L1
L18 STR



NODE ATTRIBUTES:
CONNECT IS X2 RC AT 7
CONNECT IS X2 RC AT 10
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L19 37274 SEA FILE=REGISTRY SUB=L3 SSS FUL L18

100.0% PROCESSED 52883 ITERATIONS 37274 ANSWERS
SEARCH TIME: 00.00.01

(FILE 'CAPLUS' ENTERED AT 09:53:15 ON 07 FEB 2005)
L20 13830 S L19
L21 3262 S L20(L)(RACT OR RCT)/RL
L22 39 S L21(L)PHARM?/RL

L22 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 13 Jan 2005
ACCESSION NUMBER: 2005:29314 CAPLUS
TITLE: Preparation of heterocylic 2-trifluoromethylpentan-2-

ols and related compounds as anti-inflammatory agents
INVENTOR(S): Berger, Markus; Baeurle, Stefan; Rehwinkel, Hartmut; Schmees, Norbert; Schaecke, Heike; Lehmann, Manfred; Krolikiewicz, Konrad; Schottelius, Arndt J. B.; Nguyen, Duy; Mengel, Anne; Jaroch, Stefan
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005003098	A1	20050113	WO 2004-EP6765	20040622
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10330358	A1	20050203	DE 2003-10330358	20030701
PRIORITY APPLN. INFO.:			DE 2003-10330358 A	20030701
			DE 2003-10346939 A	20031006

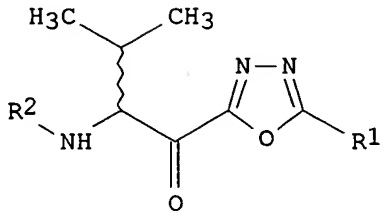
AB Title compds. I [A = aryl, benzyl, phenylethyl, etc.; R1, R2 = H, Me, Et, etc.; R3 = (un)substituted alkoxy, alkyl, alkenyl, etc.; B = Me, Et, (un)substituted methylene, etc.; Q = (un)substituted quinazoline, quinoxaline, indazole, etc.] and their pharmaceutically acceptable salts were prepared For example, palladium medaited hydrogenation of imine II, e.g., prepared from 4-(5-fluoro-2-methoxyphenyl)-2-hydroxy-4-methyl-2-trifluoromethylpentanal and 5-amino-2-methylquinazoline, afforded trifluoromethylpentanol III. In a glucocorticoid receptor binding assay, compound III exhibited an IC50 value of 1.8 nM. Compds. I are claimed to be useful as anti-inflammatory agents.
IT INDEXING IN PROGRESS
IT **825653-48-3P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(preparation of heterocylic trifluoromethylpentanols and related compds. as anti-inflammatory agents)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 16 Sep 2004
ACCESSION NUMBER: 2004:753404 CAPLUS
DOCUMENT NUMBER: 141:277626

TITLE: Preparation of oxadiazole derivatives as elastase inhibitors
INVENTOR(S): Torisu, Kazuhiko; Kobayashi, Kaoru; Naganawa, Atsushi; Sekioka, Tomohiko; Kawabata, Kazuhito
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 207 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004256473	A2	20040916	JP 2003-50563	20030227
PRIORITY APPLN. INFO.:			JP 2003-50563	20030227

OTHER SOURCE(S): MARPAT 141:277626
GI



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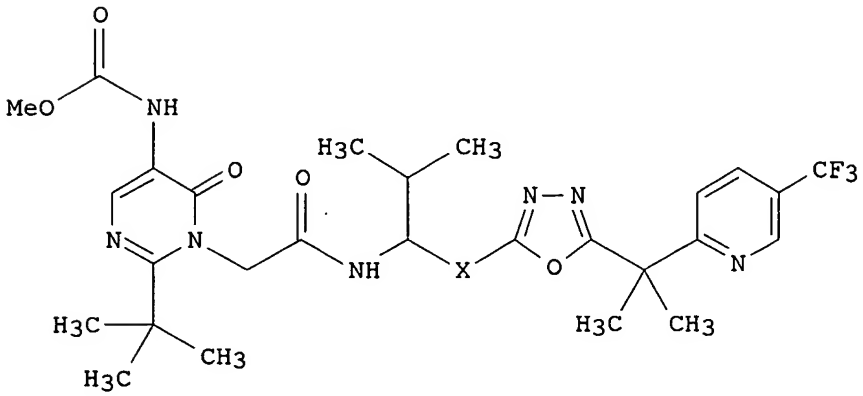


II

AB Title compds. I [R1 = monocyclic carbocycle, etc.; R2 = COR12, etc.; R12 = alkyl, etc.] were prepared For example, oxidation of compound II [X = CH(OH)], e.g., prepared from 2-chloro-5-(trifluoromethyl)pyridine in 7 steps, using Dess-Martin reagent gave compound II [X = CO]. In elastase inhibition assays, the IC50 values of compds. I were ≤10 μM. Compds. I are claimed useful for the treatment of chronic articular rheumatism, myocardial infarction, etc. Formulations are given.

IT **757970-18-6P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(preparation of oxadiazole derivs. as elastase inhibitors for treatment of
chronic articular rheumatism and myocardial infarction)

L22 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 08 Jul 2004
ACCESSION NUMBER: 2004:546414 CAPLUS
DOCUMENT NUMBER: 141:89103
TITLE: Preparation of arylquinazolines and related derivatives for promoting the release of parathyroid hormone
INVENTOR(S): Altmann, Eva; Beerli, Rene; Gerspacher, Marc; Renaud, Johanne; Weiler, Sven; Widler, Leo
PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 190 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056365	A2	20040708	WO 2003-EP14741	20031222
WO 2004056365	A3	20040819		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SY, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR

PRIORITY APPLN. INFO.: GB 2002-30015 A 20021223
OTHER SOURCE(S): MARPAT 141:89103
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

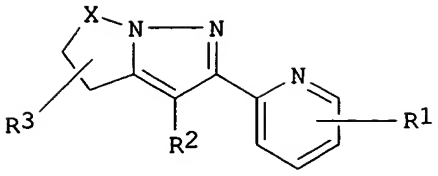
AB Title compds. I [Y = O, S; R1 = OH, SH, halo, NO2, etc.; R2 = halo, alkyl, alkenyl, etc.; R3 = alkyl, benzyl, etc.] are prepared For instance, (2-amino-5-((propargyl)oxy)phenyl)(4-isopropylphenyl)methanone is alkylated with 6-bromomethyl-2,3-dimethoxyquinoxaline (dioxane, K2CO3, 80°, 2 days) and the resulting intermediate treated with sodium isocyanate to give II. Compds. of the invention have IC50 in the range of 10 nM to 50 μM for the parathyroid calcium-sensing receptor. I are useful for treating bone conditions associated with increased calcium depletion or resorption.
IT **717103-60-1P**, [2-[[(2,3-Dimethoxyquinoxalin-6-yl)methyl]amino]-5-((prop-2-ynyl)oxy)phenyl](4-isopropylphenyl)methanone

RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(arylquinazoline and related derivs. for promoting the release of parathyroid hormone)

L22 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 18 Jun 2004
ACCESSION NUMBER: 2004:493706 CAPLUS
DOCUMENT NUMBER: 141:54330
TITLE: Preparation of novel fused pyrazoles, in particular pyrrolopyrazoles, as transforming growth factor-β (TGF-β) signal transduction inhibitors
INVENTOR(S): Beight, Douglas Wade; Burkholder, Timothy Paul; Decollo, Todd Vincent; Godfrey, Alexander Glenn; Heap, Charles Raymond; King, Chi-Hsin Richard; Li, Hong-Yu; McMillen, William Thomas; Sawyer, Jason Scott; Wang, Yan; Diefenbacher, Clive Gideon; Engler, Thomas Albert; Malhotra, Sushant; Mundla, Sreenivasa Reedy
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 143 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004050659	A1	20040617	WO 2003-US35969	20031124
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2002-429982P P 20021127
OTHER SOURCE(S): MARPAT 141:54330
GI



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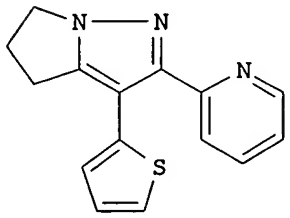


II

AB Title compds. I [wherein X = (CH2)n; n = 0-4; R1 = (un)substituted alk(en/yn)yl, alk(enyl/ynyl)oxy, alkylthio, alkylamino, alkanoyl, alkylcarbamoyl, thiophenyl, Ph, etc.; R2 = (un)substituted thiophenyl, oxazolyl, pyrazinyl, furanyl, imidazo[1,2-a]pyridinyl, benzoimidazolyl, quinoxalinyl, pyrazolo[1,5-a]pyrimidinyl, [1,8]naphthyridinyl, etc.; R3 = H, alkyl; and their pharmaceutically acceptable salts] were prepared as transforming growth factor-β (TGF-β) signal transduction inhibitors. II was prepared in 5 steps by Claisen condensation of Et pyridin-2-carboxylate, condensation of β-carbonyl ester with 1-aminopyrrolidin-2-one•HCl, cyclization in the presence of NaOEt in toluene, decarboxylative bromination, and Pd-cross coupling of the bromide with thiophene-2-boronic acid. Selected I inhibited the TGF-β type I receptor kinase domain with IC50 values < 20 μM. I are useful for treating fibroproliferative diseases associated with TGF-β1 over production

IT **705263-39-4P**, 7-[2-(6-Methylpyridin-2-yl)-5,6-dihydro-4H-pyrrolo[1,2-b]pyrazol-3-yl]-1H-quinoxalin-2-one **705263-74-7P**, 2-Chloro-7-[2-(6-methylpyridin-2-yl)-5,6-dihydro-4H-pyrrolo[1,2-b]pyrazol-3-yl]quinoxaline
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(TGF-β signal transduction inhibitor; preparation of fused pyrazoles, in particular pyrrolopyrazoles, as TGF-β signal transduction inhibitors)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 28 May 2004
ACCESSION NUMBER: 2004:433750 CAPLUS
DOCUMENT NUMBER: 141:7131
TITLE: Preparation of quinazolines and analogs as Akt

	inhibitors and indoles as protein kinase inhibitors for use in synergistic combination therapy for the treatment of cancer
INVENTOR(S):	Barnett, Stanley F.; Defeo-Jones, Deborah D.; Hartman, George D.; Huber, Hans E.; Stirdivant, Steven M.; Heimbrook, David C.
PATENT ASSIGNEE(S):	USA
SOURCE:	U.S. Pat. Appl. Publ., 121 pp., which CODEN: USXXCO
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004102360	A1	20040527	US 2003-678565		20031003
PRIORITY APPLN. INFO.:			US 2002-422312P	P	20021030
			US 2003-460911P	P	20030407

OTHER SOURCE(S): MARPAT 141:7131
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to methods of treating cancer using a combination of at least two Akt inhibitors I [wherein Q = (un)substituted heterocyclyl, aryl; U, V, W, and X = independently CH, N; Y, Z = independently CH, N, provided that at least one of Y and Z = N; n = 0-3; p = 0-2; q = 0-4; R1, R2, R7 = independently halo, CN, OH, CHO, NO2, or (un)substituted (cyclo)alkyl(oxy), alkenyl(oxy), alkynyl(oxy), heterocyclyl(oxy), acyl, carboxy, carbamoyl(oxy), ureido, sulfamoyl, etc.; R3, R4 = independently H, (perfluoro)alkyl; or CR3R4 = cycloalkyl, heterocyclyl; and pharmaceutically acceptable salts or stereoisomers thereof] or a combination of I and a protein kinase inhibitor II [wherein G = H2, O; X = C, N, SO0-2, O; m = 0-2; n = 0-2; p = 0-6; q = 0-4; R1 = independently H, halo, or (un)substituted (cyclo)alkyl, heterocyclyl, aryl, carbamoyl, amino, acyl, sulfamoyl, carboxy, etc.; R2 = H or (un)substituted (cyclo)alkyl(oxy), amino, aryloxy, heterocyclyloxy, alkenyloxy, alkynyloxy, etc.; R5 = independently H, halo, NO2, CN, or (un)substituted alkyl, alkenyl, alkynyl, carboxy, acyl, sulfamoyl, carbamoyl, ureido, amino, etc.; and pharmaceutically acceptable salts or stereoisomers thereof], optionally in combination with a third compound Examples include syntheses for I and II and assays demonstrating Akt inhibitor activity, antitumor activity, and the synergistic effect of combinations of AKT inhibitors and/or protein kinase inhibitors on caspase 3 activity. For instance, III•HCl was prepared in an 8-step reaction sequence culminating with the cycloaddn. of 4-(2-aminoprop-2-yl)benzil and o-phenylenediamine using glacial acetic acid in H2O, followed by work up with chloroform and ethanolic HCl. III•HCl, a selective Akt1 and Akt2 inhibitor, demonstrated a 3.2-fold in caspase 3 activation over control compared to a 1.2-fold increase for a protein kinase inhibitor. Combination treatment produced a 9-fold increase in caspase 3 activation.

IT **612847-29-7P 612848-47-2P**

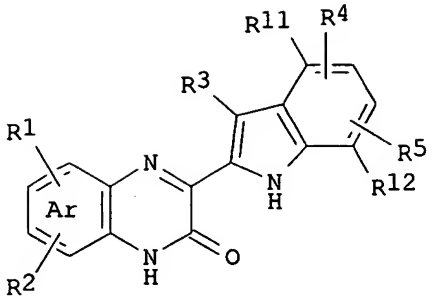
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(antitumor agent; preparation of quinazolines and analogs as Akt inhibitors
and indoles as protein kinase inhibitors for use in synergistic combination therapy for treatment of cancer)

L22 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 27 May 2004
ACCESSION NUMBER: 2004:430796 CAPLUS
DOCUMENT NUMBER: 141:7139
TITLE: Preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis
INVENTOR(S): Ladouceur, Gaetan H.; Bear, Brian; Bi, Cheng; Brittelli, David R.; Burke, Michael J.; Chen, Gang; Cook, James; Dumas, Jacques; Sibley, Robert; Turner, Michael R.
PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA
SOURCE: PCT Int. Appl., 217 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043950	A1	20040527	WO 2003-US36003	20031110
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:		
US 2002-425490P	P	20021112
US 2003-460915P	P	20030407
US 2003-484202P	P	20030630

OTHER SOURCE(S): MARPAT 141:7139
GI



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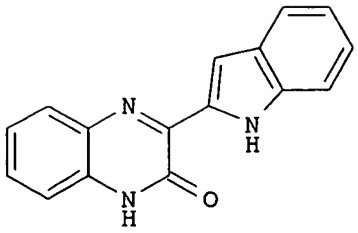


II

AB The invention relates to title compds. I [wherein Ar = 6-membered aromatic ring containing 0-2 N atoms; R1 and R2 = independently H, halo, CF3, acyl, piperidinyl, piperazinyl, morpholinyl, or (un)substituted alkyl, alkoxy, amino, pyrrolidinyl, Ph, etc.; R3 = H, alkyl, OH, NO2, NH2, alkylamino, alkoxyamino, or (un)substituted benzoylamino; R4 = H, OH, halo, CN, acyl, sulfamoyl, trialkylsiloxy, tetrazolyl, thienyl, pyrrolyl, pyrimidinyl, oxazolyl, furanyl, or (un)substituted alkyl, alkenyl, alkynyl, alkoxy, amino, oxadiazolyl, Ph, pyridyl(oxy), carbamoyl; R11 and R12 = independently H, F, or Cl with the proviso that when one of R11 and R12 = F or Cl, the other must be H; and pharmaceutically acceptable salts and esters thereof]. The invention also relates to the use of I and their pharmaceutical compns. for treating hyperproliferative disorders and diseases associated with angiogenesis (no data). Examples include representative syntheses for compds. of the invention, pharmaceutical compns. comprising them, and tumor model assays (no specific data given). For instance, N-Boc-indole was coupled with di-Me oxalate using t-BuLi to give tert-Bu 2-[methoxy(oxo)acetyl]-1H-indole-1-carboxylate (72%). Cyclization of the dione with 1,2-phenylenediamine in AcOH afforded the quinoxalinone II (77%).

IT **694528-79-5P 694528-80-8P 694528-84-2P**
694528-95-5P 694528-97-7P 694529-00-5P
694529-55-0P 694530-66-0P 694531-07-2P
694531-12-9P 694531-13-0P 694531-15-2P
694531-18-5P 694531-20-9P 694531-42-5P
694532-17-7P 694532-22-4P
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(antiproliferative and angiogenesis inhibitor; preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 21 May 2004
ACCESSION NUMBER: 2004:412920 CAPLUS
DOCUMENT NUMBER: 140:423590
TITLE: Preparation of 4-(phenylpiperidin-4-ylidenemethyl)benzamides for treatment of pain,

anxiety, or gastrointestinal disorders

INVENTOR(S): Brown, William; Griffin, Andrew
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.

SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041784	A1	20040521	WO 2003-SE1705	20031105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: SE 2002-3301 A 20021107
OTHER SOURCE(S): MARPAT 140:423590
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [wherein R1 = (un)substituted alkyl, cycloalkyl(alkyl), (hetero)aryl, R8CO, R8SO2, R8SO, R8NHCO, R8CS, or R8NHCS; ; R2 = H or (un)substituted alkyl; R3 = H or (un)substituted alkoxycarbonyl, alkyl, or cycloalkyl(alkyl); R8 = (un)substituted alkyl, (hetero)aryl(alkyl), or cycloalkyl(alkyl); or pharmaceutically acceptable salts thereof] were prepared as opioid δ receptor ligands. For example, reaction of 4-(bromomethyl)benzoic acid Me ester with P(OMe)3, followed by addition of 1-(tert-butoxycarbonyl)-4-piperidone in the presence of LDA in THF, gave 4-(4-methoxycarbonylbenzylidene)piperidine-1-carboxylic acid tert-Bu ester (35%). Addition of Br2 (78%) and reaction with NaOH in MeOH provided 4-[bromo(4-carboxyphenyl)methylene]piperidine-1-carboxylic acid tert-Bu ester (87%). Conversion to the benzoyl chloride with iso-Bu chloroformate and amidation (73%) with Et2NH in the presence of TEA in CH2Cl2, followed by coupling with 3-aminophenylboronic acid using Pd(PPh3)4 and Na2CO3 in toluene/EtOH/H2O afforded N,N-diethyl-4-[(3-aminophenyl)(piperidin-4-ylidene)methyl]benzamide (97%). Alkylation of the amine with benzaldehyde and NaBH(OAc)3 in 1,2-dichloroethane gave II. In binding assays using human 293S cells expressing cloned human opioid receptors and neomycin resistance, most compds. of the invention exhibited activity toward the δ receptor with IC50 values in the range of 0.14 nM - 31.2 nM. Exemplified compds. also showed some activity toward the κ and μ receptors with IC50 values in the ranges of 36 nM - 9680 nM and 3 nM - 5975 nM, resp. Thus, I and their pharmaceutical compns. are useful in therapy, in particular for the treatment of gastrointestinal disorders,

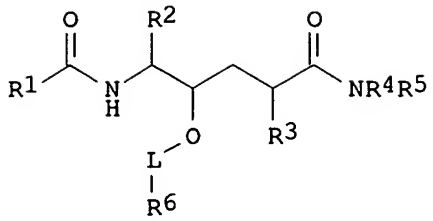
anxiety, or pain (no data).

IT **692246-95-0P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(δ receptor agonist; preparation of (phenylpiperidinylidenemethyl)benzamides as δ receptor agonists for treatment of pain, anxiety, or gastrointestinal disorders)

L22 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 13 May 2004
ACCESSION NUMBER: 2004:390233 CAPLUS
DOCUMENT NUMBER: 140:406822
TITLE: A preparation of heteroaryl-hexanoic acid amide derivatives as immunomodulatory agents
INVENTOR(S): Brown, Matthew Frank; Gaweco, Anderson See; Gladue, Ronald Paul; Kath, John Charles; Poss, Christopher Stanley
PATENT ASSIGNEE(S): Pfizer Products Inc., USA
SOURCE: PCT Int. Appl., 66 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039787	A1	20040513	WO 2003-IB4626	20031020
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004097554	A1	20040520	US 2003-687380	20031016
PRIORITY APPLN. INFO.:			US 2002-422574P P	20021030

OTHER SOURCE(S): MARPAT 140:406822
GI



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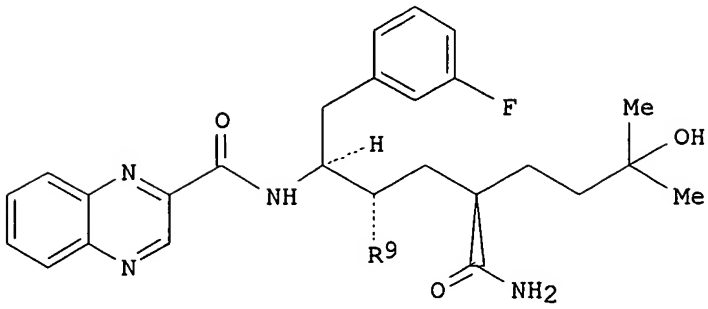


II

AB The invention relates to heteroaryl-hexanoic acid amide derivs. of formula I [wherein: R1 is a substituted heteroaryl; R2 is phenyl-(CH2)0-4, naphthyl-(CH2)0-4, or C3-C10cycloalkyl-(CH2)0-4, etc.; R3 is H, C1-10alkyl, C3-C10cycloalkyl-(CH2)0-6, (hetero)aryl-(CH2)0-6; R4 is H, alkyl, OH, alkoxy, hydroxyalkyl, alkoxy-C(O)-, etc.; R5 is H, alkyl, or amino; R4 and R5 together with the N-atom to which they are attached form (un)substituted C2-C9heterocycloalkyl; R6 is H, (HO)2P(O)-, HOS(O)2-, etc.; L is a bond or -O(CR7R8)-; R7 and R8 are independently H or C1-C3alkyl], useful as immunomodulatory agents. The invented compds. are inhibiting cell infiltration (ED50 < 30 μM). The proposed dose of the invented compds. for oral, parenteral, nasal, or buccal administration to the average adult human is 0.1 to 1 g per unit dose. The invention relates to
methods of using the above-described compds. and compns. for the treatment and prevention of diseases and conditions including those that may be treated or prevented by antagonizing the CCR1 receptor. For instance, hexanoic acid amide derivative II [R9 = OC(O)(CH2)2CO2H] was prepared via esterification of succinic anhydride by alc. II (R9 = OH).

IT **91-19-0DP**, Quinoxaline, derivs.
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(preparation of heteroaryl-hexanoic acid amide derivs. useful as immunomodulatory agents)

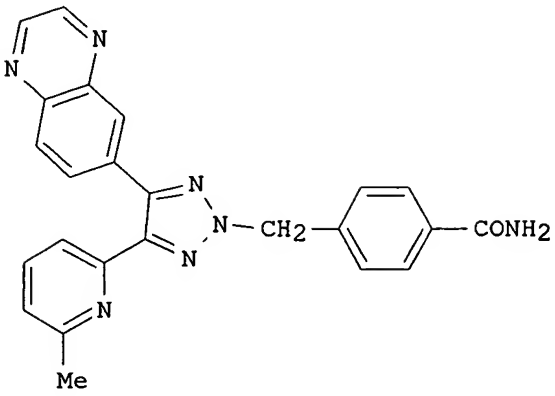
L22 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 28 Apr 2004
ACCESSION NUMBER: 2004:346231 CAPLUS
DOCUMENT NUMBER: 141:71490
TITLE: Synthesis and biological evaluation of novel

2-pyridinyl-[1,2,3]triazoles as inhibitors of transforming growth factor β1 type 1 receptor

AUTHOR(S): Kim, Dae-Kee; Kim, Joonseop; Park, Hyun-Ju
CORPORATE SOURCE: College of Pharmacy, Ewha Womans University, 11-1 Daehyun-dong, Seodaemun-gu, Seoul, 120-750, S. Korea

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2401-2405
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:71490

GI



I

AB A series of 2-pyridinyl-[1,2,3]triazoles have been synthesized and evaluated for their ALK5 inhibitory activity in the luciferase reporter assays. Quinoxalinyl-substituted 2-pyridinyl-[1,2,3]triazole I showed significant ALK5 inhibition (SBE-luciferase activity, 25%; p3TP-luciferase activity, 17%) at a concentration of 5 μM that is comparable to that of SB-431542 (SBE-luciferase activity, 21%; p3TP-luciferase activity, 12%), but weak p38α MAP kinase inhibition (13%) at a concentration of 10 μM that is much lower than that of SB-431542 (54%).

IT **710946-98-8P 710946-99-9P 710947-10-7P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation of 2-pyridinyl-[1,2,3]triazoles as inhibitors of transforming growth factor β1 type 1 receptor)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 15 Apr 2004
ACCESSION NUMBER: 2004:306973 CAPLUS
DOCUMENT NUMBER: 141:33319

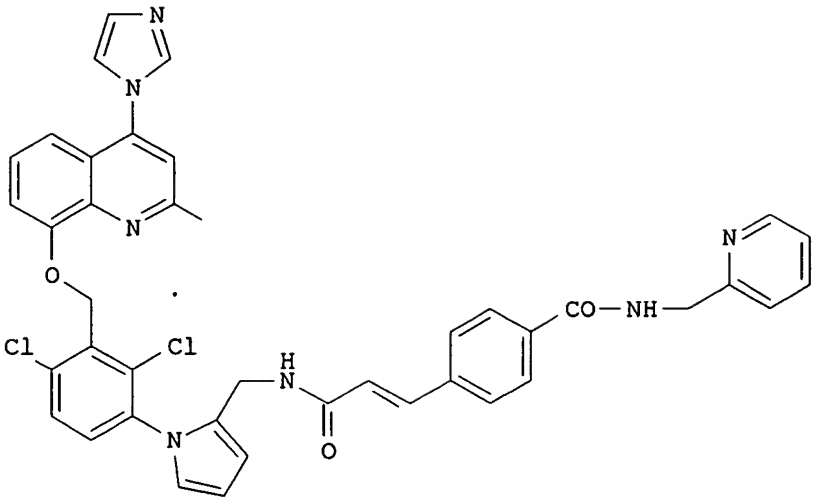
TITLE: Design, synthesis, and biological evaluation of novel 2-pyridinyl-[1,2,4]triazoles as inhibitors of transforming growth factor β1 type 1 receptor
AUTHOR(S): Kim, Dae-Kee; Kim, Joonseop; Park, Hyun-Ju
CORPORATE SOURCE: College of Pharmacy, Ewha Womans University, Seoul, 120-750, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(9), 2013-2020
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of 2-pyridinyl-[1,2,4]triazoles have been synthesized and evaluated for their ALK5 inhibitory activity in the luciferase reporter assays. Compound 12b showed significant ALK5 inhibition (SBE-Luciferase, 73%; p3TP-Luciferase, 85%) at a concentration of 5 μM that is comparable to that of SB-431542 (SBE-Luciferase, 79%; p3TP-Luciferase, 88%), but weak p38α MAP kinase inhibition (4%) at a concentration of 10 μM that is much lower than that of SB-431542 (54%). The binding mode of 12b generated by flexible docking studies revealed that the structure of 12b is a good fit into the (NPC-30345)-binding cavity of ALK5.

IT **701979-18-2P 701979-19-3P**
RL: **PAC (Pharmacological activity)**; PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(design, synthesis, and biol. evaluation of novel 2-pyridinyl-[1,2,4]triazoles as inhibitors of transforming growth factor β1 type 1 receptor)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 02 Mar 2004
ACCESSION NUMBER: 2004:168613 CAPLUS
DOCUMENT NUMBER: 140:368093
TITLE: A New Series of Highly Potent Non-Peptide Bradykinin B2 Receptor Antagonists Incorporating the 4-Heteroarylquinoline Framework. Improvement of Aqueous Solubility and New Insights into Species Difference
AUTHOR(S): Sawada, Yuki; Kayakiri, Hiroshi; Abe, Yoshito; Imai, Keisuke; Mizutani, Tsuyoshi; Inamura, Noriaki; Asano, Masayuki; Aramori, Ichiro; Hatori, Chie; Katayama, Akira; Oku, Teruo; Tanaka, Hirokazu
CORPORATE SOURCE: Exploratory Research Laboratories, Fujisawa Pharmaceutical Co. Ltd., Ibaraki, 300-2698, Japan
SOURCE: Journal of Medicinal Chemistry (2004), 47(7), 1617-1630
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



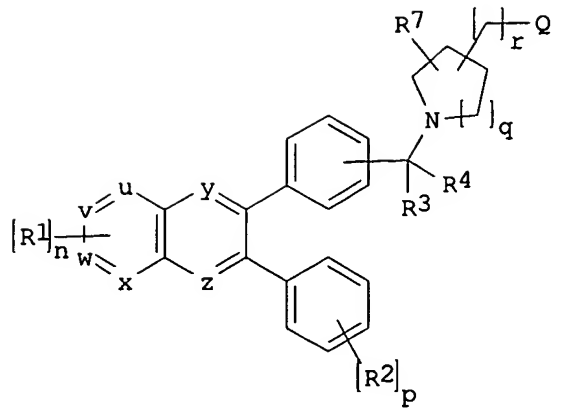
I

AB Introduction of nitrogen-containing heteroarom. groups at the 4-position of the quinoline moiety of the authors non-peptide B2 receptor antagonists resulted in enhancing binding affinities for the human B2 receptor and reducing binding affinities for the guinea pig one, providing new structural insights into species difference. A CoMFA study focused on the diversity of the quinoline moiety afforded correlative and predictive QSAR models of binding for the human B2 receptor but not for the guinea pig one. A series of 4-(1-imidazolyl)quinoline derivs. could be dissolved in a 5% aqueous solution of citric acid up to a concentration of 10 mg/mL. A representative compound (I) inhibited the specific binding of [3H]bradykinin to the cloned human B2 receptor expressed in Chinese hamster ovary cells with an IC50 value of 0.26 nM and significantly inhibited bradykinin-induced bronchoconstriction in guinea pigs even at 1 μg/kg by i.v. administration.

IT **215238-12-3 683273-27-0**
RL: **PAC (Pharmacological activity)**; PRP (Properties); **RCT (Reactant)**; THU (Therapeutic use); BIOL (Biological study); **RACT (Reactant or reagent)**; USES (Uses)
(bradykinin B2 receptor antagonists incorporating the 4-heteroarylquinoline framework and improvement of aqueous solubility and new insights into species difference in relation to bronchodilating activity)

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 12 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 29 Feb 2004
ACCESSION NUMBER: 2004:162686 CAPLUS
DOCUMENT NUMBER: 140:199493
TITLE: Preparation of novel quinuclidine derivatives for therapeutic use in the treatment of diseases or disorders responsive to modulation of cholinergic receptors and/or monoamine receptors



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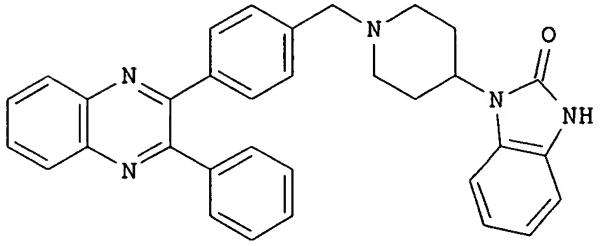

II

AB The title compds. comprising a 2,3-diphenylquinoxaline moiety [I; u, v, w and x = CH, N; y, z = CH, N (provided that at least one of y and z = N); Q = NR5R6, (un)substituted aryl, heterocyclyl; R1 = alkenyl, halo, CN, etc.; R2 = OH, CN, CO2H, etc.; R3, R4 = H, alkyl, perfluoroalkyl; or R3 and R4 are combined to form (CH2)t wherein one of the carbon atoms is optionally replaced by O, SOm, (un)substituted NHCO, N(COH); R5, R6 = H, aryl, heterocyclyl, etc.; or NR5R6 = monocyclic or bicyclic heterocycle; R7 = halo, CN, CO2H, etc.; n = 0-3; p = 0-2; t = 2-6; m = 0-2; q = 0-4; r = 0-1] and their salts which inhibit the activity of Akt, a serine/threonine protein kinase, were prepared E.g., a 2-step synthesis of the quinoxaline II [starting from 4-bromomethylbenzil and 4-(2-keto-1-benzimidazolinyl)piperidine], was given. The exemplified compds. I were found to have IC50 of ≤ 50 μM against one or more of Akt1, Akt2 and Akt3. The invention is further directed to chemotherapeutic compns. containing the compds. I and methods for treating cancer comprising administration of the compds. I.

IT **612847-29-7P 612847-31-1P 612848-75-6P 612848-76-7P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(preparation of 2,3-diphenylquinoxaline derivs. as inhibitors of Akt activity for treating cancer)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 17 Oct 2003
ACCESSION NUMBER: 2003:818232 CAPLUS
DOCUMENT NUMBER: 139:323527
TITLE: Preparation of triazolo[4,3-b]pyridazines and 2,3-diarylquinazolines for the treatment of cancer
INVENTOR(S): Barnett, Stanley F.; Defeo-Jones, Deborah; Haskell, Kathleen M.; Huber, Hans E.; Nahas, Deborah D.; Lindsley, Craig W.; Zhao, Zhijian; Hartman, George D.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003084473	A2	20031016	WO 2003-US10632	20030404
WO 2003084473	A3	20040212		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-370827P P 20020408
US 2002-417202P P 20021009

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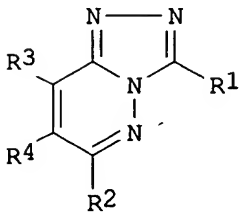

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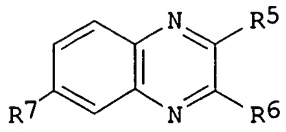

II

AB Triazolo[4,3-b]pyridazines I [R1 = (un)substituted Ph, furyl, thienyl, pyridinyl; R2 = substituted NH2, OH; R3 = H, R4 = (un)substituted cycloalkyl, aryl; R3R4 = (un)substituted CH:CHCH:CH] and quinazolines II [R5, R6 = (un)substituted Ph; R7 = H, alkyl, halogen, OH, alkoxy] were prepared for use as inhibitors of one or two of the isoforms of Akt, a serine/threonine protein kinase, acting particularly on the pleckstrin homol. domain of Akt. Thus, 3,6-dichloropyridazine was converted to its

4-cyclobutyl derivative which was cyclized with BzNHNH2 and aminated to give I
[R1 = Ph, R2 = NHCH2CMe2CH2NMe2, R3 = H, R4 = cyclobutyl]. This compound had IC50 for inhibition of Akt1 of 1.4 μM.

IT **612847-30-0P 612847-32-2P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(preparation of triazolo[4,3-b]pyridazines and 2,3-diarylquinazolines for the treatment of cancer)

L22 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 26 Aug 2003
ACCESSION NUMBER: 2003:665554 CAPLUS
DOCUMENT NUMBER: 139:285655
TITLE: Potent quinoxaline-based inhibitors of PDGF receptor tyrosine kinase activity. Part 2: the synthesis and biological activities of RPR127963, an orally bioavailable inhibitor
AUTHOR(S): He, Wei; Myers, Michael R.; Hanney, Barbara; Spada, Alfred P.; Bilder, Glenda; Galzcinski, Helen; Amin, Dilip; Needle, Saul; Page, Ken; Jayyosi, Zaid; Perrone, Mark H.
CORPORATE SOURCE: Aventis Pharmaceuticals, Brigdewater, NJ, 08807, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(18), 3097-3100
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:285655
AB RPR127963 demonstrates an excellent pharmacokinetic profile in several species and was found to be efficacious in the prevention of restenosis in a Yucatan mini-pig model upon oral administration of 1-5 mg/kg. The in vitro selectivity profile and SAR of the highly optimized PDGF-R tyrosine kinase inhibitor are highlighted.

IT **217093-53-3P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent);** USES (Uses)
(synthesis and PDGF receptor tyrosine kinase-inhibiting activity of RPR127963 and its derivs.)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 01 Aug 2003
ACCESSION NUMBER: 2003:591177 CAPLUS
DOCUMENT NUMBER: 139:149652
TITLE: Preparation of 2-acylaminothiazole derivatives or salts thereof as c-Mpl receptor ligands
INVENTOR(S): Sugasawa, Keizo; Watanuki, Susumu; Koga, Yuji; Nagata, Hiroshi; Obitsu, Kazuyoshi; Wakayama, Ryutaro; Hirayama, Fukushi; Suzuki, Ken-ichi

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003062233	A1	20030731	WO 2003-JP270	20030115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1466912	A1	20041013	EP 2003-700571	20030115
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.: JP 2002-10413 A 20020118
JP 2002-10447 A 20020118
WO 2003-JP270 W 20030115

OTHER SOURCE(S): MARPAT 139:149652

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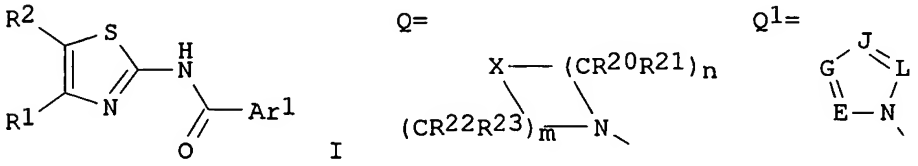

AB 2-Acylaminothiazole derivs. or pharmaceutically acceptable salts thereof [I; Ar1 = each (un)substituted aryl, monocyclic aromatic heterocyclyl, or bicyclic condensed heterocyclyl; R1 = each (un)substituted aryl or monocyclic aromatic heterocyclyl; R2 = Q, Q1, R24R25N; wherein n, m = an integer of 1-3; when n or m is an integer of ≥2, CR20R21 and CR22R23 may represent a different group; X = O, S, NR26, C(R27)R28; E, G, J, L = N, CR29; R20-R23, R26-R29 = H, OH, lower alkoxy, each (un)substituted lower alkyl, cycloalkyl, aryl, arylalkyl, aromatic heterocyclyl, aromatic heterocyclylalkyl, nonarom. heterocyclyl, lower alkenyl, lower alkylidene, NH2, or CONH2, CO2H, lower alkoxycarbonyl, lower alkenyloxycarbonyl, aryl-lower alkoxycarbonyl, aromatic heterocyclyl-lower alkoxycarbonyl, lower alkylcarbonylamino, oxo; R24, R25 = H, each (un)substituted lower alkyl, cycloalkyl, or nonarom. heterocyclyl] are prepared These compds. have an excellent effect of proliferating human c-Mpl-Ba/F3 cells and an activity of increasing platelets (thrombocytosis) based on the effect of promoting the formation

of megakaryocytic colonies and are useful in treating thrombopenia. Thus, 2.1 mL Et isonipecotinate was added to a solution of 750 mg 5,6-dichloro-N-[4-(4-chlorothiophen-2-yl)-5-(4-cyclohexylpiperazin-1-yl)thiazol-2-yl]nicotinamide in 10 mL THF, heated to 50°, and stirred for 5 h to give, after workup and silica gel chromatog., 881 mg 1-[3-chloro-5-[[4-(4-chlorothiophen-2-yl)-5-(4-cyclohexylpiperazin-1-yl)thiazol-2-yl]carbamoyl]-2-pyridyl]piperidine-4-carboxylic acid Et ester which (30 mg) was dissolved in 1 mL MeOH, treated with 0.12 mL 1 M aqueous NaOH solution at room temperature, stirred for 24 h, distilled under reduced pressure, dissolved in EtOAc, treated with 0.2 mL 1 M aqueous HCl solution, stirred, and distilled under reduced pressure, followed by washing the residue with Et2O to give 20 mg 1-[3-chloro-5-[[4-(4-chlorothiophen-2-yl)-5-(4-cyclohexylpiperazin-1-yl)thiazol-2-yl]carbamoyl]-2-pyridyl]piperidine-4-carboxylic acid hydrochloride (II). II and recombinant human thrombopoietin (rhTPO) at 2.4 ad 0.012 nM, resp., showed 30% of the maximum cell proliferating effect of each compound tested on human c-Mpl-Ba/F3 cell.

IT **570405-07-1P**
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(preparation of 2-acylaminothiazole derivs. or salts thereof as c-Mpl receptor ligands for proliferating human c-Mpl-Ba/F3 cells and increasing platelets via promoting the formation of megakaryocytic colony)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 30 May 2003
ACCESSION NUMBER: 2003:412773 CAPLUS
DOCUMENT NUMBER: 139:381448
TITLE: Some reactions with ketene dithioacetals. Part II: Novel synthesis of quinoxaline, pyrazole and pyrrolo[3,4-b]quinoxaline derivatives using ketene dithioacetals as antimicrobial activity
AUTHOR(S): El-Sharief, A. M. Sh.; Zahran, M. A.; El-Gaby, M. S. A.; Ammar, Y. A.; El-Said, U. H.
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo, Egypt
SOURCE: Afinidad (2003), 60(503), 81-87
CODEN: AFINAE; ISSN: 0001-9704
PUBLISHER: Asociacion de Quimicos del Instituto Quimico de Sarria
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:381448

AB The key compound, [(4-aminophenylaminomethylthio)methylene]malonitrile (I) was synthesized by condensation of ketene dithioacetals and 1,4-phenylenediamine. The reactivity of quinoxaline-2,3-dicarboxylic anhydride (II) towards compound I as nitrogen nucleophile was investigated. Thus, treatment of compound II with I in refluxing ethanol afforded the quinoxaline carboxylic acid derivative (III). On the other hand, fusion of compound II and I at 160°C yielded the corresponding quinoxaline carboxamide (IV). Fusion of compds. III and IV with hydrazine hydrate at

150°C produced the novel corresponding substituted pyrazoles. Refluxing of compound III with acetic anhydride furnished the novel pyrrolo[3,4-b]quinoxaline. By treatment of compound I with aromatic sulfonyl chloride followed by fusion with hydrazine, the novel pyrazole was obtained. The anti-microbial activity of some selected compound was also reported.

IT **623934-58-7P 623934-59-8P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**
(ring closure of; multi-step preparation of quinoxaline, pyrazole and pyrroloquinoxaline derivs. using ketene dithioacetals and their antimicrobial activity)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 07 Mar 2003
ACCESSION NUMBER: 2003:174477 CAPLUS
DOCUMENT NUMBER: 138:226731
TITLE: Alpha-2-adrenergic agonist/fatty acid compositions
INVENTOR(S): Woodward, David F.; Ambrus, Gyorgy
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 13 pp., Cont.-in-part of U.S. Pat. Appl. 2002 198,210.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003045524	A1	20030306	US 2002-136263	20020501
US 2002198210	A1	20021226	US 2001-848249	20010503
PRIORITY APPLN. INFO.:			US 2001-848249 A2	20010503

AB Compns. comprising an alpha-2-adrenergic agonist component and a fatty acid component, that enhances the pharmacokinetic disposition of the therapeutic component, are disclosed. The fatty acid component may include linolenic acid and/or other fatty acids. A brimonidine-linoleic acid complex was formed and its effect on intraocular pressure determined

IT **59803-98-4**, Brimonidine **91147-43-2**, 6-Quinoxalinamine, N-(4,5-dihydro-1H-imidazol-2-yl)- **474777-33-8**
RL: **PAC (Pharmacological activity); RCT (Reactant);** THU (Therapeutic use); BIOL (Biological study); **RACT (Reactant or reagent)**; USES (Uses)
(α2-adrenergic agonist/fatty acid compns.)

L22 ANSWER 25 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 07 Feb 2003
ACCESSION NUMBER: 2003:97401 CAPLUS
DOCUMENT NUMBER: 138:153554
TITLE: Preparation of quinoline and quinoxaline derivatives as inhibitors of factor Xa with therapeutic uses
INVENTOR(S): Schmitt, Martine; Klotz, Evelyne; Macher, Jean-Paul;

Bourguignon, Jean-Jacques
PATENT ASSIGNEE(S): NEURO3D, Fr.
SOURCE: PCT Int. Appl., 283 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003010146	A1	20030206	WO 2002-FR2594	20020719
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2827599	A1	20030124	FR 2001-9730	20010720
EP 1451159	A1	20040901	EP 2002-790206	20020719
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				

PRIORITY APPLN. INFO.: FR 2001-9730 A 20010720
WO 2002-FR2594 W 20020719

OTHER SOURCE(S): MARPAT 138:153554
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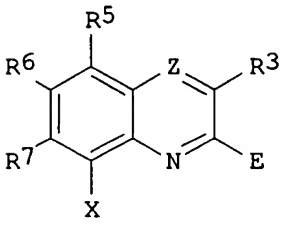


I

AB The invention concerns compds. quinoline and quinoxaline derivs. (shown as I; variables defined below; e.g. 4,8-dihydroxy-5,7-dichloroquinoline-2-carboxylic acid), their preparation and their uses, in particular in therapeutic treatments and vaccines or for developing active compds. For I: E = COOH, COOR1, CH2OH, CHO, CH2COOH, CH2COOR1, C(O)NHR2, or 1H-tetrazol-5-yl; R1 = (C1-C12)alkyl or (C6-C18)aryl(C1-C12)alkyl; R2 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, hydroxy; R3 = H, halo, hydroxy, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl or (C3-C17)heteroaryl. Z = N or CR4; R4 = H, (C1-C12)alkyl, (C2-C12)alkyn-1-yl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, OR8, NR9R9, (C1-C17)heteroaryl or (C2-C12)alken-1-yl; R5, R6 and R7 = H, halo, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl , NR9R9', COR10, (C2-C12)alken-1-yl, (C2-C12)alkyn-1-yl, (C1-C17)heteroaryl, (C3-C17)heteroaryl(C1-C12)alkyl, cyano or nitro; -R8 = H, (C1-C12)alkyl,

(C6-C18)aryl(C1-C12)alkyl. R9 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, acyl, tert-butoxycarbonyl, (C1-C17)heteroaryl or (C6-C18)arylsulfonyl or (C1-C12)alkylsulfonyl; R9', which may be same or different than R9 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, acyl, tert-butoxycarbonyl, (C1-C17)heteroaryl or (C6-C18)arylsulfonyl or (C1-C12)alkylsulfonyl; NR9R9' = cycloheteroalkyl: N(CH2)m(CH2)nY (n = 2 or 3, m = 2 or 3 and Y = CH2, SO2, or NR11, O, S); R10 = H, (C1-C12)alkyl or (C6-C18)aryl or NHR2. R11 = H, (C1-C12)alkyl, (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, (C1-C17)heteroaryl, (C1-C17)heteroaryl(C1-C12)alkyl or COR10; X = halo, OR8, NR9R9', (C6-C18)aryl, (C6-C18)aryl(C1-C12)alkyl, (C3-C12)alkyl, (C2-C12)alken-1-yl, (C2-C12)alkyn-1-yl, (C1-C17)heteroaryl, COR10, cyano or nitro; addnl. details are given in the claims. Test results for inhibition of factor Xa by .apprx.50 examples of I are included; for example, 4,8-dihydroxy-5,7-dichloroquinoline-2-carboxylic acid exhibits IC50 = 4.6 μM and 163 % of the inhibitory activity of xanthurenic acid at 10 μM. More than 100 example prepns. of I are included. For example, Me 4-hydroxy-6-bromo-8-methoxyquinoline-2-carboxylate was prepared in 64% yield from Me 2-[(4-bromo-2-methoxyphenyl)amino]but-2-enedioate in Ph2O at 250° for 5-15 min; the reactant was prepared in 93% yield from 2-methoxy-4-bromoaniline and Me acetylenedicarboxylate in MeOH at reflux for 1 h.

IT **495407-42-6P**, Ethyl 8-hydroxy-3-oxo-3,4-dihydroquinoxaline-2-carboxylate **495407-43-7P**, Ethyl 8-(benzyloxy)-3-oxo-3,4-dihydroquinoxaline-2-carboxylate **495407-45-9P**, Ethyl [8-(benzyloxy)-3-oxo-3,4-dihydroquinoxaline-2(1H)-ylidene]acetate
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(drug candidate; preparation of quinoline and quinoxaline derivs. as inhibitors of factor Xa with therapeutic uses)

REFERENCE COUNT: 87 THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 11 Dec 2002
ACCESSION NUMBER: 2002:939992 CAPLUS
DOCUMENT NUMBER: 139:270356
TITLE: Comparative study of isoflavone, quinoxaline and oxindole families of anti-angiogenic agents
AUTHOR(S): Whatmore, Jacqueline L.; Swann, Elizabeth; Barraja, Paola; Newsome, Jeffery J.; Bunderson, Melisa; Beall, Howard D.; Tooke, John E.; Moody, Christopher J.
CORPORATE SOURCE: School of Sport and Health Sciences, University of Exeter, Exeter, EX4 4QD, UK
SOURCE: Angiogenesis (2002), 5(1-2), 45-51
CODEN: AGIOFT; ISSN: 0969-6970
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:270356

AB A study designed to compare the effects on VEGF-induced angiogenesis of a number of known anti-angiogenic agents together with some novel derivs. thereof was undertaken. Thus the isoflavone biochanin A (1), indomethacin (2), the 3-arylquinoxaline SU1433 and its derivs. (3-6), the benzoic acid

derivative (7), the oxindoles SU5416 (8) and SU6668 (11), together with their simple N-benzyl derivs. (9, 10, and 12) were selected for study. Using an in vitro assay the compds. were evaluated for their ability to inhibit VEGF-induced angiogenesis in HUVECs, and the cytotoxicity of representative compds. was also studied in tumor cell lines using 24-h exposure. The results indicate that the SU compds., SU1433, SU5416 and SU6668, are more potent inhibitors of VEGF-induced angiogenesis than indomethacin or the naturally occurring biochanin A, presumably because they inhibit VEGF receptor signaling. Blocking one of the phenolic OH groups of SU1433 reduced anti-angiogenic activity, as did blocking the NH groups of SU5416 and SU6668. Cytotoxicity studies indicate that none of the compds. examined exhibited cytotoxicity at anti-angiogenic concns.

IT **168835-90-3P**, SU 1433
RL: DMA (Drug mechanism of action); **PAC (Pharmacological activity)**; PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(preparation and comparative study of isoflavone, quinoxaline and oxindole families of anti-angiogenic agents)

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

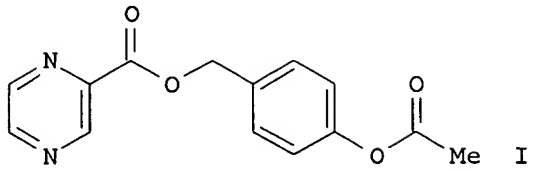
L22 ANSWER 27 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 03 Dec 2002
ACCESSION NUMBER: 2002:917077 CAPLUS
DOCUMENT NUMBER: 139:36744
TITLE: A versatile synthetic route to chiral quinoxaline derivatives from amino acids precursors
AUTHOR(S): El-Faham, Ayman; El Massry, Abdel Moneim; Amer, Adel; Gohar, Yousry M.
CORPORATE SOURCE: Faculty of Science, Chemistry Department, University of Alexandria, Alexandria, Egypt
SOURCE: Letters in Peptide Science (2002), 9(1), 49-54
CODEN: LPSCEM; ISSN: 0929-5666
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:36744

AB The synthesis of N-protected L-amino acid (3-benzylquinoxalin-2-yl)hydrazide derivs. is reported. 3-Benzyl-2-hydrazinoquinoxaline was prepared and then coupled with N-Boc-L-amino acids, including alanine, valine, leucine, phenylalanine, tyrosine, serine and proline, in the presence of HBTU as a coupling reagent to provide the expected product with high yield and purity. The products were deprotected by p-toluenesulfonic acid in acetonitrile and the tosylate salts were evaluated for antibacterial and antifungal activity.

IT **223929-23-5P**
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**
(synthesis of L-amino acid (benzylquinoxalinyl)hydrazide derivs. and their antibacterial and antifungal activities)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 07 Nov 2002
ACCESSION NUMBER: 2002:844381 CAPLUS
DOCUMENT NUMBER: 138:73233
TITLE: Synthesis and Antimycobacterial Activity of Pyrazine and Quinoxaline Derivatives
AUTHOR(S): Seitz, Lainne E.; Suling, William J.; Reynolds, Robert C.
CORPORATE SOURCE: Organic Chemistry Department and Biochemistry Department, Southern Research Institute, Birmingham, AL, 35255-5305, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(25), 5604-5606
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:73233
GI



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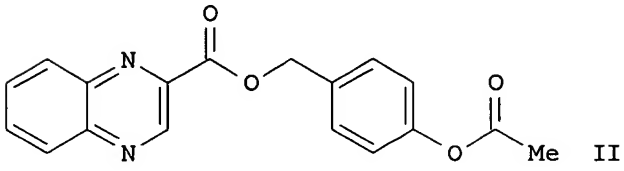

II

AB A series of pyrazine and quinoxaline derivs. have been synthesized, and their activity against M. tuberculosis (Mtb) and Mycobacterium avium (MAC) are reported. The 4-acetoxybenzyl ester of pyrazinoic acid (I) and 4'-acetoxybenzyl 2-quinoxalinecarboxylate (II) showed excellent activity against Mtb (MIC ranges of less than 1-6.25 μg/mL) but only modest activity against MAC (MICs of 4-32 μg/mL).

IT **1865-11-8P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation, antitubercular activity, and structure-activity relationship
of alkyl and benzyl quinoxalinecarboxylates via coupling of alcs. with quinoxalinecarbonyl chloride)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 17 Oct 2002
ACCESSION NUMBER: 2002:790220 CAPLUS
DOCUMENT NUMBER: 137:294982
TITLE: Preparation of piperazinylpyrazinyl aryloxyalkyl ethers as 5-HT2C receptor agonists
INVENTOR(S): Nilsson, Bjorn; Tejbrant, Jan; Pelcman, Benjamin; Ringberg, Erik; Thor, Markus; Nilsson, Jonas; Jonsson, Mattias
PATENT ASSIGNEE(S): Biovitrum AB, Swed.
SOURCE: U.S., 45 pp., Cont.-in-part of U.S. Ser. No. 573,348, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6465467	B1	20021015	US 2000-589282	20000608
ZA 2001009571	A	20021120	ZA 2001-9571	20011120
US 2003092694	A1	20030515	US 2002-269670	20021011
US 6759401	B2	20040706		
US 2004242554	A1	20041202	US 2004-873852	20040622

PRIORITY APPLN. INFO.:
SE 1999-1884 A 19990521
US 1999-137527P P 19990603
US 2000-573348 B2 20000519
US 2000-589282 A3 20000608
US 2002-269670 A1 20021011

OTHER SOURCE(S): MARPAT 137:294982
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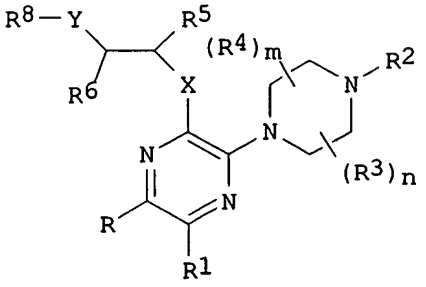

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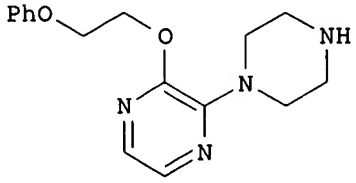


II

AB The title compds. (I) [wherein X and Y = independently O, S, or NR7; R and R1 = independently H, alkyl, or halo; or C2RR1 = optionally halo substituted benzene or thiophene; R2 = H, OH, or alkyl; R3, R4, and R5 = independently H or alkyl; R6 = H or alkyl; or CYR6R8 for a 5-6 membered heterocycle; R7 = H or alkyl, preferably Me or Et; R8 = (un)substituted (hetero)aryl; m and n = independently 1 or 2; or pharmaceutically

acceptable salts, hydrates, geometric isomers, tautomers, optical isomers, N-oxides, and prodrugs thereof] were prepared and tested as 5-HT2C receptor agonists. For instance, 2,3-dichloropyrazine and 2-phenoxyethanol were treated with t-BuONa in dioxane to give 2-chloro-3-(2-phenoxyethoxy)pyrazine (62%). The halopyrazine, piperazine, and K2CO3 in MeCN were stirred and heated to afford the desired 2-(phenoxy)ethyl 3-(1-piperazinyl)-2-pyrazinyl ether (II) in 65% yield, which was then converted to the maleate salt. In competition expts., I showed affinity for 5-HT2C receptor protein with Ki values typically ranging from 1 nM to 1500 nM and specific values ranging from 5 nM to 377 nM for twelve compds. I exhibited agonist efficacy at the 5-HT2C receptor by mobilizing intracellular Ca in transfected HEK293 cells with maximum responses in the range of 20-100% relative to the maximum response of 5-HT (serotonin) at a concentration of 1 μM. Acute toxicity studies in mice following oral administration of I showed that mortality typically occurred at doses between 200 mg/kg to 450 mg/kg body weight I are useful for the treatment of serotonin-related central nervous system disorders, such as eating disorders, memory disorders, schizophrenia, mood disorders, anxiety disorders, pain, sexual dysfunctions, and urinary disorders (no data).

IT **313654-02-3P**, 2-(2-Phenoxyethoxy)-3-(1-piperazinyl)quinoxaline **313656-86-9P**, 2-[2-(3-Pyridinyloxy)ethoxy]-3-(1-piperazinyl)quinoxaline **313656-92-7P**, 2-[2-(3-Pyridinyloxy)ethoxy]-3-(1-piperazinyl)-6,7-dichloroquinoxaline
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(preparation of heterocyclylpyrazinyl aryloxyalkyl ether 5-HT2C receptor agonists from aryloxyalkanols, halopyrazines, and heterocycles)

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 29 Jul 2002
ACCESSION NUMBER: 2002:558411 CAPLUS
DOCUMENT NUMBER: 137:257239
TITLE: SAR by MS: A Ligand Based Technique for Drug Lead Discovery Against Structured RNA Targets
AUTHOR(S): Swayze, Eric E.; Jefferson, Elizabeth A.; Sannes-Lowery, Kristin A.; Blyn, Lawrence B.; Risen, Lisa M.; Arakawa, Satoshi; Osgood, Stephen A.; Hofstadler, Steven A.; Griffey, Richard H.
CORPORATE SOURCE: Ibis Therapeutics, A Division of Isis Pharmaceuticals Inc., Carlsbad, CA, 92008, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(18), 3816-3819
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:257239

AB A technique for lead discovery vs. RNA targets utilizing mass spectrometry (MS) screening methods is described. The structure-activity relationships (SAR) derived from assaying weak binding motifs allows the pharmacophores discovered to be elaborated via "SAR by MS" to higher affinity ligands.

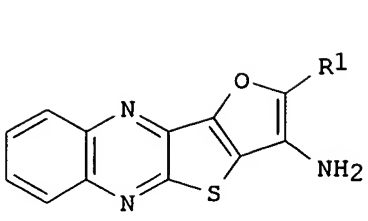
Application of this strategy to a subdomain of the 23S rRNA afforded a new class of compds. with functional activity.

IT **14121-55-2**
RL: CST (Combinatorial study, unclassified); **PAC (Pharmacological activity)**; **RCT (Reactant)**; THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); **RACT (Reactant or reagent)**; USES (Uses)
(SAR by MS: ligand-based technique for drug lead discovery against structured RNA targets)

IT **462119-65-9P 462119-66-0P 462119-67-1P 462119-68-2P 462119-69-3P**
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(SAR by MS: ligand-based technique for drug lead discovery against structured RNA targets)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 11 Apr 2002
ACCESSION NUMBER: 2002:271488 CAPLUS
DOCUMENT NUMBER: 137:78924
TITLE: Synthesis and antimicrobial activity of novel furothienoquinoxalines, pyranothienoquinoxalines and pyrimidopyranothienoquinoxalines
AUTHOR(S): Moustafa, Osama S.; El-Ossaily, Yasser A.
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Assiut University, Assiut, 71516, Egypt
SOURCE: Journal of the Chinese Chemical Society (Taipei, Taiwan) (2002), 49(1), 107-112
CODEN: JCCTAC; ISSN: 0009-4536
PUBLISHER: Chinese Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:78924
GI



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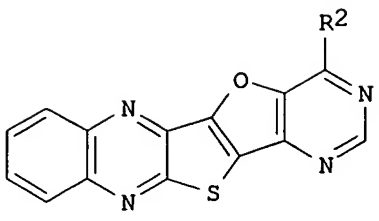

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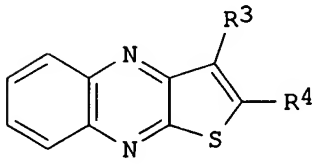
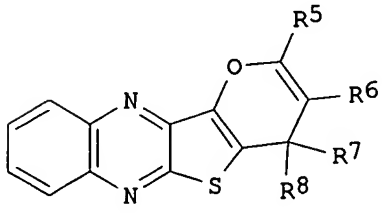


III



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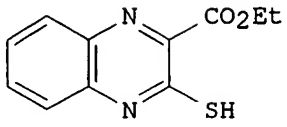


V

AB Furothienoquinoxalines I (R1 = CN, COOEt) and II (R2 = HO, NH2), thienoquinoxalines III (R3 = HO, EtO2CCH2O; R4 = H, CN), and pyranothienoquinoxalines IV (R5 = EtO2C, EtO2CCH:N, MeCONH; R6 = H, CN; R7 = Ph, R8 = H; R7R8 = O) were prepared by multi-step synthesis from mercaptoquinoxaline V and tested against Gram pos. and Gram neg. bacteria and fungi. Most of I-IV showed good growth inhibition against Gram pos. bacteria, while III (R3 = HO, R4 = H) was active against all types of bacteria and fungi studied.

IT **278186-19-9**
RL: **PAC (Pharmacological activity); RCT (Reactant);** BIOL (Biological study); **RACT (Reactant or reagent)**
(preparation of antibacterial and antifungal thienoquinoxalines via cyclocondensation of ethoxycarbonyl(mercapto)quinoxaline with α-halo ketones and esters)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 02 Apr 2002
ACCESSION NUMBER: 2002:246597 CAPLUS
DOCUMENT NUMBER: 137:134476
TITLE: Anti-Mycobacterium tuberculosis agents derived from quinoxaline-2-carbonitrile and quinoxaline-2-carbonitrile 1,4-di-N-oxide
AUTHOR(S): Ortega, Miguel Angel; Sainz, Yolanda; Montoya, Maria Elena; Jaso, Andres; Zarranz, Belen; Aldana, Ignacio; Monge, Antonio
CORPORATE SOURCE: Unidad en Investigacion y Desarrollo de Medicamentos, CIFA, Universidad de Navarra, Pamplona, Spain
SOURCE: Arzneimittel-Forschung (2002), 52(2), 113-119

CODEN: ARZNAD; ISSN: 0004-4172
PUBLISHER: Editio Cantor Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:134476

AB In this paper new quinoxaline derivs. with different substituents in positions 3, 6, 7 and 8 are reported. Their biol. activities against Mycobacterium tuberculosis have been assessed and most of the 1,4-di-N-oxide derivs. have been shown to strongly inhibit the bacteria growth in the first in vitro screening. One of these N-oxides (4) is a promising candidate due to its good Selectivity Index (7.95). On the other hand, those compds. without N-oxide moieties showed no or very low activity (growth inhibition: 17% and 39%).

IT **444807-95-8P**
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(quinoxaline-2-carbonitrile derivs. anti-Mycobacterium tuberculosis action)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 20 Mar 2002
ACCESSION NUMBER: 2002:211240 CAPLUS
DOCUMENT NUMBER: 137:226178
TITLE: 5-Phosphonomethylquinoxalinediones as competitive NMDA receptor antagonists with a preference for the human 1A/2A, rather than 1A/2B receptor composition
AUTHOR(S): Auberson, Yves P.; Allgeier, Hans; Bischoff, Serge; Lingenhoehl, Kurt; Moretti, Robert; Schmutz, Markus
CORPORATE SOURCE: Novartis Pharma AG, Basel, 4002, Switz.
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(7), 1099-1102
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:226178

AB NMDA antagonists derived from 5-phosphonomethyl-1,4-dihydroquinoxaline-2,3-dione are potent anticonvulsant agents, and display strong protective effects in the electroshock-induced convulsion assay in mice. Their preference for the human NMDAR 1A/2A over 1A/2B subunit composition was optimized, leading to compound (1RS,1'S)-PEAQX, which shows a >100-fold selectivity.

IT **459836-14-7P 459836-15-8P**
RL: **PAC (Pharmacological activity)**; PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(5-phosphonomethylquinoxalinediones as competitive NMDA receptor antagonists with a preference for human 1A/2A, rather than 1A/2B receptor composition)

IT **187479-25-0 187479-26-1 459836-02-3 459836-07-8 459836-08-9 459836-09-0**

459836-22-7
RL: **PAC (Pharmacological activity)**; PRP (Properties); **RCT (Reactant)**; THU (Therapeutic use); BIOL (Biological study); **RACT (Reactant or reagent)**; USES (Uses)
(5-phosphonomethylquinoxalinediones as competitive NMDA receptor antagonists with a preference for human 1A/2A, rather than 1A/2B receptor composition)
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 15 Feb 2002
ACCESSION NUMBER: 2002:119100 CAPLUS
DOCUMENT NUMBER: 138:83
TITLE: Quinoxaline chemistry. Part 14. 4-(2-Quinoxalylamino)-phenylacetates and 4-(2-quinoxalylamino)-phenylacetyl-l-glutamates as analogues-homologues of classical antifolate agents. Synthesis and evaluation of in vitro anticancer activity
AUTHOR(S): Piras, Sandra; Loriga, Mario; Paglietti, Giuseppe
CORPORATE SOURCE: Dipartimento Chimico Tossicologico, Universita di Sassari, Sassari, 07100, Italy
SOURCE: Farmaco (2002), 57(1), 1-8
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:83
AB Among a new series of 26 4-(3-substituted-2-quinoxalylamino)phenylacetates and 4-(3-substituted-2-quinoxalylamino)phenylacetyl-l-glutamates, eight were selected at NCI for evaluation of their in vitro anticancer activity. The results obtained in comparison with the corresponding nor-compds. series seem to indicate that this type of homologation is not helpful.
IT **476374-02-4P 476374-03-5P 476374-04-6P**
476374-05-7P 476374-06-8P 476374-07-9P
476374-08-0P 476374-09-1P 476374-10-4P
476374-11-5P 476374-12-6P 476374-13-7P
476374-14-8P 476374-15-9P 476374-16-0P
476374-17-1P 476374-18-2P 476374-27-3P
RL: DMA (Drug mechanism of action); **PAC (Pharmacological activity)**; PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(quinoxaline chemical and synthesis and evaluation of in vitro anticancer activity)
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

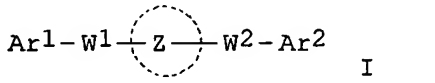
L22 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 10 Feb 2002
ACCESSION NUMBER: 2002:107312 CAPLUS
DOCUMENT NUMBER: 136:167389
TITLE: Preparation of pyrrole, indole, thiophene, pyrazole, imidazole, and isothiazole derivatives as inhibitors of transforming growth factor-beta (TGF-β)
INVENTOR(S): Tokunaga, Teruhisa; Hume, William Ewan; Kitoh, Makoto;

Nagata, Ryu
PATENT ASSIGNEE(S): Sumitomo Pharmaceuticals Co., Ltd., Japan
SOURCE: PCT Int. Appl., 215 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002010131	A1	20020207	WO 2001-JP6495	20010727
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001075794	A5	20020213	AU 2001-75794	20010727
CA 2416946	AA	20030122	CA 2001-2416946	20010727
EP 1310485	A1	20030514	EP 2001-953325	20010727
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2003181496	A1	20030925	US 2003-352067	20030128
US 6759429	B2	20040706		
US 2004209939	A1	20041021	US 2004-840746	20040507

PRIORITY APPLN. INFO.:
JP 2000-229423 A 20000728
WO 2001-JP6495 W 20010727
US 2003-352067 A3 20030128

OTHER SOURCE(S): MARPAT 136:167389
GI



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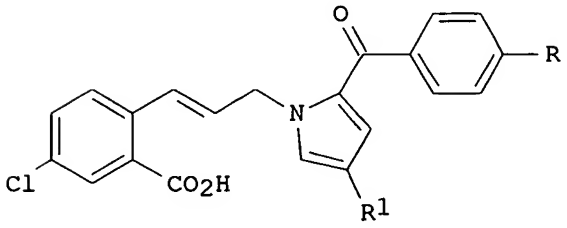


III

AB The title compds. represented by the following formula (I) or pharmaceutically acceptable salts of these [wherein ring Z represents an optionally substituted pyrrole, indole, thiophene, pyrazole, benzene, imidazole, or isothiazole; W2 represents CO, SO2, CONR (R = H, alkyl), optionally substituted C1-4 alkylene or C2-4 alkenylene; Ar2 represents

optionally substituted aryl or heteroaryl; and W1 and Ar1 mean the following: (1) W1 represents optionally substituted C1-4 alkylene or C2-4 alkenylene, Ar1 represents bicyclic heteroaryl having one to four N atoms or (2) W1 represents optionally substituted C2-5 alkylene, C2-5 alkenylene, C2-5 alkynylene, or -Y-W3 (wherein Y = O or cycloalkanediyl; W3 = optionally substituted C1-5 alkylene, C2-5 alkenylene, or C2-5 alkynylene), Ar represents optionally substituted aryl or monocyclic heteroaryl substituted at ortho or meta position by CO2H, alkoxycarbonyl, optionally alkyl-substituted carbamoyl, cyclic aminocarbonyl, alkylsulfonylcarbonyl, arylsulfonylcarbonyl, alkylsulfonyl, etc.] or prodrugs or pharmacol. acceptable salts thereof are prepared These compds. are useful as fibroid inhibitors for organs or tissues. Thus, bromination of 3-(4-chloro-2-methoxycarbonylphenyl)-2-propenol (preparation given) by N-bromosuccinimide and PPh3 in CH2Cl2 at 0° for 10 min gave 3-(4-chloro-2-methoxycarbonylphenyl)-2-propenyl bromide (II). A THF solution of 2-(4-methylbenzoyl)pyrrole was added dropwise to a suspension of NaH in THF and the resulting solution was slowly added dropwise to a THF solution of II at 55° and stirred for 2 h to give 2-[3-[2-(4-methylbenzoyl)-1-pyrrolyl]-1-propen-1-yl]-5-chlorobenzoic acid Me ester which was saponified with aqueous NaOH in methanol and acidified with aqueous HCl to give III (R = Me, R1 = H). In a kidney fibroid model using a rat Thy-1 nephritis model, administration of III.Na (R = Me, R1 = H) at 15 mg/kg and Thy-1 (one of surface antigens of thymocyte) to rats lowered the level of hydroxyproline (fibroid index) in kidney compared to the control group administered only with Thy-1. III.Na (R = 2-morpholinoethoxy, R1 = Me) at 3 μM in vitro inhibited the TGF-β-induced production of proteoglycan in MRK-49F rat fibroblast cells by 99%.

IT **397323-98-7P**, 8-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397324-06-0P**, 5-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397324-14-0P**, 6-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397324-20-8P**, 7-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline **397325-01-8P**, 2-[[2-(4-Hydroxybenzoyl)pyrrol-1-yl]methyl]quinoxaline **397325-03-0P**, 2-[[2-(4-((Ethoxycarbonyl)methoxy)benzoyl)pyrrol-1-yl]methyl]quinoxaline
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(preparation of pyrrole, indole, thiophene, pyrazole, imidazole, and isothiazole derivs. as inhibitors of transforming growth factor-β and fibroid inhibitors for organs or tissues)

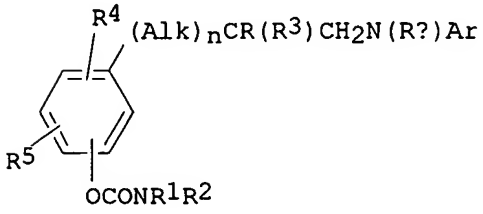
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 01 Feb 2002
ACCESSION NUMBER: 2002:90040 CAPLUS
DOCUMENT NUMBER: 136:135022
TITLE: Preparation of heteroaryl-β-alanine derivatives as antiinflammatory agents and α4 integrin inhibitors
INVENTOR(S): Konradi, Andrei W.; Pleiss, Michael A.; Thorsett,

Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Semko, Christopher; Xu, Ying-Zi
PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; American Home Products Corporation
SOURCE: PCT Int. Appl., 141 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008222	A2	20020131	WO 2001-US23096	20010720
WO 2002008222	A3	20020613		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002086882	A1	20020704	US 2001-910431	20010719
PRIORITY APPLN. INFO.:			US 2000-220128P P	20000721

OTHER SOURCE(S): MARPAT 136:135022
GI



I

AB Disclosed are a series of heteroaryl-β-alanine derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted aromatic or heteroarom. group, as well as their

pharmaceutical use as α4β7 Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepared as α4 Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the α4β1 and αaβ7 assays of 1 μM and below. In the other assays featuring α integrins of other subgroups the same compds. had IC50 values of 50 μM and above thus demonstrating the potency and selectivity of their action against α4 integrins. Title compds. were prepared for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.

IT **263275-09-8P 263275-11-2P**
RL: IMF (Industrial manufacture); **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(preparation of heteroaryl-β-alanine derivs. as antiinflammatory agents and α4 integrin inhibitors)

L22 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 01 Feb 2002
ACCESSION NUMBER: 2002:90026 CAPLUS
DOCUMENT NUMBER: 136:135019
TITLE: Preparation of 3-amino-2-(4-aminocarbonyloxy)phenyl-propionic acid derivatives as antiinflammatory agents and α4 Integrin inhibitors
INVENTOR(S): Konradi, Andrei W.; Pleiss, Michael A.; Thorsett, Eugene D.; Ashwell, Susan; Welmaker, Gregory S.; Kreft, Anthony; Sarantakis, Dimitrios; Dressen, Darren B.; Grant, Francine S.; Xu, Ying-Zi
PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; American Home Products Corporation
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

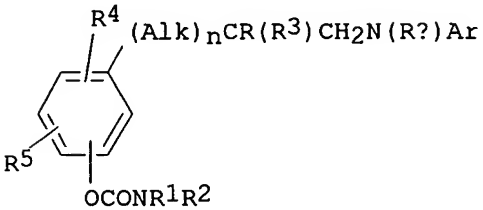
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008206	A1	20020131	WO 2001-US23073	20010720

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2002055509	A1	20020509	US 2001-910685	20010720
US 6689781	B2	20040210		
US 2004127486	A1	20040701	US 2003-735499	20031212
PRIORITY APPLN. INFO.:			US 2000-220134P	P 20000721
			US 2001-910685	A3 20010720

OTHER SOURCE(S): MARPAT 136:135019

GI



I

AB 3-Amino-2-(4-aminocarbonyloxy)phenyl-propionic acid derivs. I wherein R is a carboxylic acid; R1 and R2 are independently selected from the group consisting of hydrogen, alkyl, substituted alkyl, alkenyl, substituted alkenyl, cycloalkyl, substituted cycloalkyl, or R1 and R2, together with the nitrogen atom to which they are attached, are joined to form an optionally substituted heterocyclic ring provided that said substituted alkyl, substituted alkenyl and substituted cycloalkyl do not carry an aryl, substituted aryl, heteroaryl or substituted heteroaryl group; Ra and R3 are independently a hydrogen or a Me group; R4 and R5 are independently selected from the group consisting of heteroatom group; n is zero or an integer 1; Alk is a straight or branched alkylene chain; Ar is an optionally substituted aromatic or heteroarom. group, as well as their pharmaceutical use as α4β7 Integrin inhibitors for the treatment of inflammatory diseases. Thus, 3-[4-(3,5-dichloropyrid-4-ylcarboxamido)phenyl]-2-(3-chlorophenylamino)propanoic acid was prepared as α4 Integrin inhibitor. The preferred compds. of the invention generally have IC50 values in the α4β1 and αaβ7 assays of 1 μM and below. In the other assays featuring α integrins of other subgroups the same compds. had IC50 values of 50 μM and above thus demonstrating the potency and selectivity of their action against α4 integrins. Title compds. were prepared for treating an inflammatory condition in a mammalian patient which condition is mediated by Very Late Antigen 4 (VLA-4). Inflammatory condition is selected from the group consisting of asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, multiple sclerosis, rheumatoid arthritis, tissue transplantation, tumor metastasis, meningitis, encephalitis, stroke, nephritis, retinitis, atopic dermatitis, psoriasis, myocardial ischemia and acute leukocyte-mediated lung injury.

IT **263275-09-8P 263275-11-2P**

RL: IMF (Industrial manufacture); **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)

(preparation of aminoaminocarbonyloxyphenylpropionic acid derivs. as a integrin inhibitors)

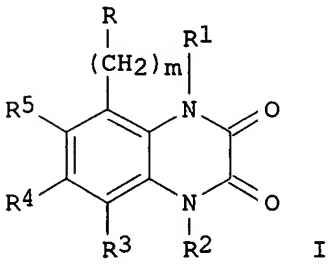
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 24 Jan 2002
ACCESSION NUMBER: 2002:66864 CAPLUS
DOCUMENT NUMBER: 136:118473
TITLE: Preparation of conformationally semi-constrained quinoxaline-2,3-diones as neuroprotective agents
INVENTOR(S): Kornberg, Brian Edward; Nikam, Sham Shridhar; Rafferty, Michael Francis
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: U.S., 27 pp., Cont.-in-part of U.S. Ser. No. 25,295, now abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

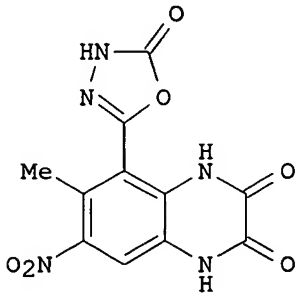
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6340758	B1	20020122	US 1998-199627	19981125
US 2002065415	A1	20020530	US 2001-971237	20011004
US 6455698	B2	20020924		

PRIORITY APPLN. INFO.: US 1997-46626P P 19970516
US 1998-25295 B2 19980213
US 1998-199627 A3 19981125

OTHER SOURCE(S): MARPAT 136:118473
GI



I



II

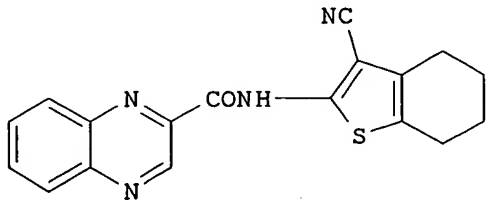
AB Title compds. I [wherein R = (un)substituted azacyclo, substituted carboxamido, piperazinocarbonyl, or diazepanylcarbonyl; R2 = H; R3 = H; R4 = independently H, (cyclo)alkyl, alkenyl, halo(alkyl), NO2, CN, SO2CF3, CH2SO2R7, (CH2)mCO2R7, (CH2)mCONR7R8, (CH2)mSO2NR8R9, or NHCOR7; R7, R8, and R9 = independently H, (cyclo)alkyl, haloalkyl, or (CH2)mR11; R11 = alkyl, alkoxy, OH, or NH2; m = 0-4; or pharmaceutically acceptable salts thereof], as well as 2,3-dimethoxyquinoxaline-5-carboxamides, were prepared as neuroprotective agents. For example, cycloaddn. of di-Me oxalate with 2,3-diamino-6-methylbenzoic acid Me ester (6-step preparation from anthranilic acid given) afforded 6-methyl-2,3-dioxo-1,2,3,4-tetrahydroquinoxaline-5-carboxylic acid Me ester (69%). Nitration (97%), followed by hydrazide formation (80%) and cycloaddn. with phosgene (50%), afforded

6-methyl-7-nitro-5-(5-oxo-4,5-dihydro-[1,3,4]oxadiazol-2-yl)-1,4-dihydroquinoxaline-2,3-dione (II). The latter exhibited strong excitatory amino acid antagonizing properties at the AMPA binding site on the AMPA glutamate receptor.

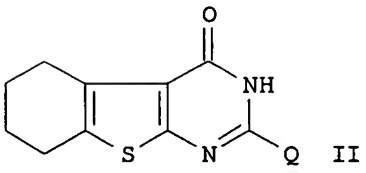
IT **258508-93-9P**, [(2,3-Dimethoxy-6-methyl-7-nitroquinoxaline-5-carbonyl)amino]acetic acid tert-butyl ester
RL: **PAC (Pharmacological activity)**; **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**; USES (Uses)
(neuroprotective agent; preparation of conformationally semi-constrained quinoxalinediones and dimethoxyquinoxalinecarboxamides as neuroprotective agents)

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

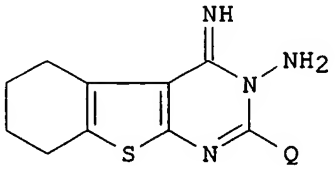
L22 ANSWER 39 OF 39 CAPLUS COPYRIGHT 2005 ACS on STN
ED Entered STN: 13 May 2001
ACCESSION NUMBER: 2001:340055 CAPLUS
DOCUMENT NUMBER: 136:102343
TITLE: Synthesis and anticancer activity of some novel 2-(quinoxalin-2-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidine derivatives
AUTHOR(S): Ismail, M. M. F.; Zahran, Medhat A.; El-Gaby, M. S. A.; Ammar, Y. A.
CORPORATE SOURCE: Chemistry Department, Faculty of Pharmacy (Girl's), Al-Azhar University, Nasr City, Egypt
SOURCE: Al-Azhar Bulletin of Science (1999), 10(1), 41-50
CODEN: ABSCE7; ISSN: 1110-2535
PUBLISHER: Al-Azhar University, Faculty of Science
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:102343
GI



I



II



III

AB 2-Carboxamide derivative I was obtained by a fusion reaction and refluxing of

I in acetic anhydride afforded thieno[2,3-d]pyrimidine II (Q = 2-quinoxalinyl). Cyclization of the intermediate I with hydrazine hydrate in refluxing butanol furnished a thieno[2,3-d]pyrimidine derivative III (Q = 2-quinoxalinyl). Reaction of III with aromatic aldehydes led to the formation of Schiff's bases. A thiourea derivative was obtained by refluxing of III with Ph isothiocyanate in pyridine. Preliminary pharmacol. screening revealed that some of the new compds. exhibited anticancer activity.

IT **389085-71-6P 389085-74-9P 389085-81-8P**
RL: **PAC (Pharmacological activity); RCT (Reactant);** SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and anticancer activity of (quinoxalinyl)tetrahydrobenzo[4,5]thieno[2,3-d]pyrimidine derivs.)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

E1 THROUGH E131 ASSIGNED

FILE 'REGISTRY' ENTERED AT 09:54:59 ON 07 FEB 2005

L23 131 SEA FILE=REGISTRY ABB=ON PLU=ON (263275-09-8/BI OR 263275-11-2/BI OR 612847-29-7/BI OR 14121-55-2/BI OR 168835-90-3/BI OR 1865-11-8/BI OR 187479-25-0/BI OR 187479-26-1/BI OR 215238-12-3/BI OR 217093-53-3/BI OR 223929-23-5/BI OR 258508-93-9/BI OR 278186-19-9/BI OR 313654-02-3/BI OR 313656-86-9/BI OR 313656-92-7/BI OR 389085-71-6/BI OR 389085-74-9/BI OR 389085-81-8/BI OR 397323-98-7/BI OR 397324-06-0/BI OR 397324-14-0/BI OR 397324-20-8/BI OR 397325-01-8/BI OR 397325-03-0/BI OR 444807-95-8/BI OR 459836-02-3/BI OR 459836-07-8/BI OR 459836-08-9/BI OR 459836-09-0/BI OR 459836-14-7/BI OR 459836-15-8/BI OR 459836-22-7/BI OR 462119-65-9/BI OR 462119-66-0/BI OR 462119-67-1/BI OR 462119-68-2/BI OR 462119-69-3/BI OR 474777-33-8/BI OR 476374-02-4/BI OR 476374-03-5/BI OR 476374-04-6/BI OR 476374-05-7/BI OR 476374-06-8/BI OR 476374-07-9/BI OR 476374-08-0/BI OR 476374-09-1/BI OR 476374-10-4/BI OR 476374-11-5/BI OR 476374-12-6/BI OR 476374-13-7/BI OR 476374-14-8/BI OR 476374-15-9/BI OR 476374-16-0/BI OR 476374-17-1/BI OR 476374-18-2/BI OR 476374-27-3/BI OR 495407-42-6/BI OR 495407-43-7/BI OR 495407-45-9/BI OR 570405-07-1/BI OR 59803-98-4/BI OR 612847-30-0/BI OR 612847-31-1/BI OR 612847-32-2/BI OR 612848-47-2/BI OR 612848-75-6/BI OR 612848-76-7/BI OR 623583-65-3/BI OR 623934-58-7/BI OR 623934-59-8/BI OR 642478-38-4/BI OR 643069-13-0/BI OR 643069-72-1/BI OR 643069-97-0/BI OR 643070-09-1/BI OR 643070-52-4/BI OR 643070-54-6/BI OR 659729-63-2/BI OR 659729-66-5/BI OR 659729-73-4/BI OR 663191-50-2/BI OR 681235-15-4/BI OR 681235-17-6/BI OR 683273-27-0/BI OR 692246-95-0/BI OR 694528-79-5/BI OR 694528-80-8/BI OR 694528-84-2/BI OR 694528-95-5/BI OR 694528-97-7/BI OR 694529-00-5/BI OR 694529-55-0/BI OR 694530-66-0/BI OR 694531-07-2/BI OR 694531-12-9/BI OR 694531-13-0/BI OR 694531-15-2/BI OR 694531-18-5/BI OR 694531-

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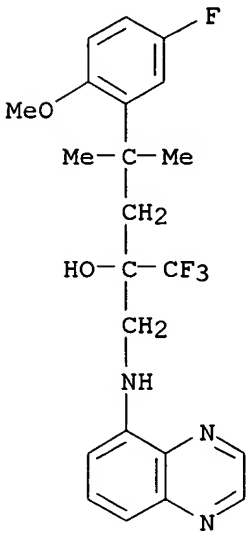
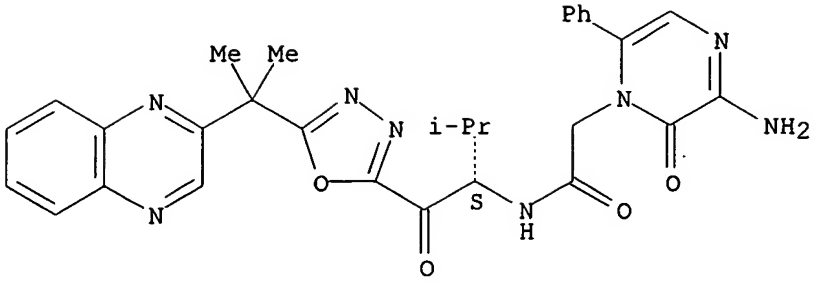
L23 ANSWER 1 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **825653-48-3** REGISTRY
CN INDEX NAME NOT YET ASSIGNED
MF C22 H23 F4 N3 O2
SR CA
LC STN Files: CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L23 ANSWER 2 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **757970-18-6** REGISTRY
CN 1(2H)-Pyrazineacetamide, 3-amino-N-[(1S)-2-methyl-1-[[5-[1-methyl-1-(2-quinoxalinyl)ethyl]-1,3,4-oxadiazol-2-yl]carbonyl]propyl]-2-oxo-6-phenyl-(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H30 N8 O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.

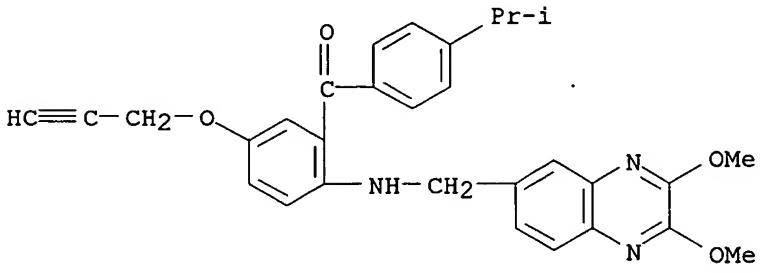


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:277626

L23 ANSWER 3 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **717103-60-1** REGISTRY
CN Methanone, [2-[[(2,3-dimethoxy-6-quinoxalinyl)methyl]amino]-5-(2-propynyloxy)phenyl][4-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN [2-[[(2,3-Dimethoxyquinoxalin-6-yl)methyl]amino]-5-((prop-2-ynyl)oxy)phenyl](4-isopropylphenyl)methanone
FS 3D CONCORD
MF C30 H29 N3 O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

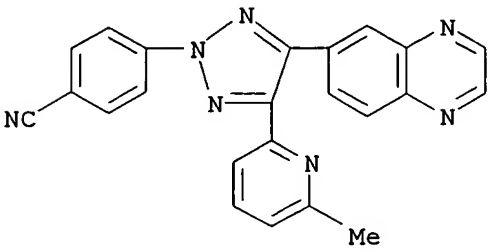


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:89103

L23 ANSWER 4 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **710947-10-7** REGISTRY
CN Benzonitrile, 4-[4-(6-methyl-2-pyridinyl)-5-(6-quinoxalinyl)-2H-1,2,3-triazol-2-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H15 N7
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

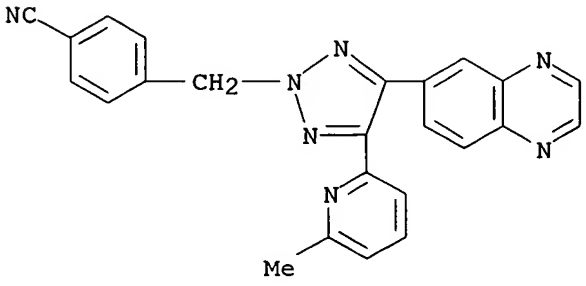


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:71490

L23 ANSWER 5 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **710946-99-9** REGISTRY
CN Benzonitrile, 4-[[4-(6-methyl-2-pyridinyl)-5-(6-quinoxalinyl)-2H-1,2,3-triazol-2-yl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H17 N7
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)



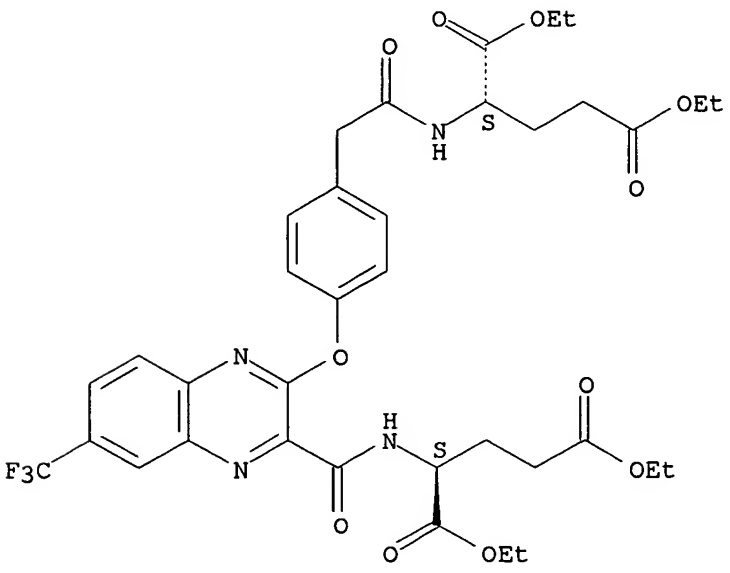
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:71490

L23 ANSWER 7 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **709638-58-4** REGISTRY
CN L-Glutamic acid, N-[[4-[[3-[[[(1S)-4-ethoxy-1-(ethoxycarbonyl)-4-oxobutyl]amino]carbonyl]-6-(trifluoromethyl)-2-quinoxalinyl]oxy]phenyl]acetyl]-, diethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C36 H41 F3 N4 O11
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.

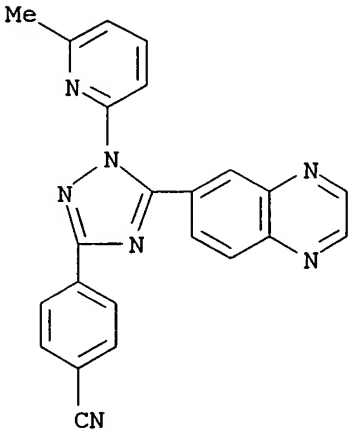


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:64522

L23 ANSWER 25 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **701979-19-3** REGISTRY
CN Benzonitrile, 4-[1-(6-methyl-2-pyridinyl)-5-(6-quinoxalinyl)-1H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H15 N7
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

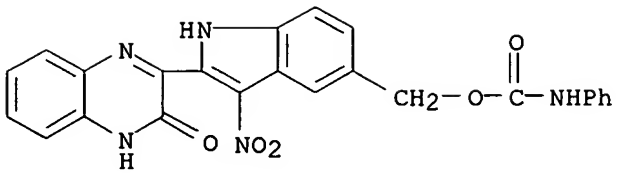


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:33319

L23 ANSWER 27 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **694532-22-4** REGISTRY
CN 2(1H)-Quinoxalinone, 3-[3-nitro-5-[[[(phenylamino)carbonyl]oxy]methyl]-1H-indol-2-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H17 N5 O5
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

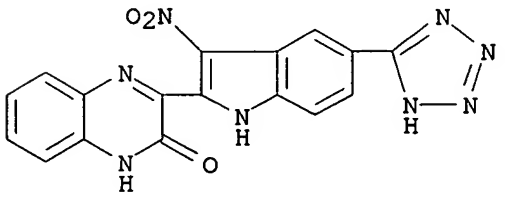


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 29 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **694531-42-5** REGISTRY
CN 2(1H)-Quinoxalinone, 3-[3-nitro-5-(1H-tetrazol-5-yl)-1H-indol-2-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H10 N8 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



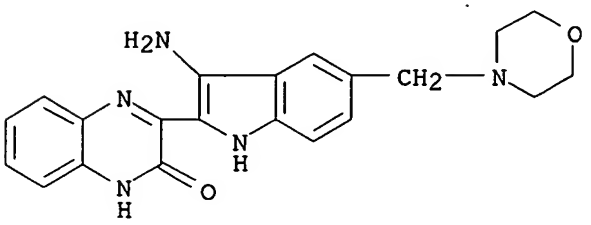
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 36 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **694530-66-0** REGISTRY
CN 2(1H)-Quinoxalinone, 3-[3-amino-5-(4-morpholinylmethyl)-1H-indol-2-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H21 N5 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

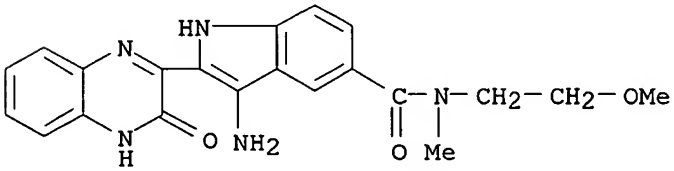


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 37 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **694529-55-0** REGISTRY
CN 1H-Indole-5-carboxamide, 3-amino-2-(3,4-dihydro-3-oxo-2-quinoxalinyl)-N-(2-methoxyethyl)-N-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H21 N5 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



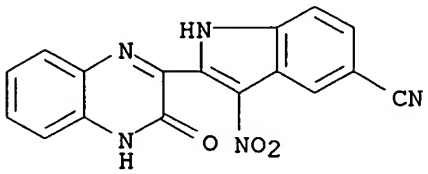
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 39 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **694528-97-7** REGISTRY
CN 1H-Indole-5-carbonitrile, 2-(3,4-dihydro-3-oxo-2-quinoxalinyl)-3-nitro- (9CI) (CA INDEX NAME)
FS 3D CONCORD

MF C17 H9 N5 O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

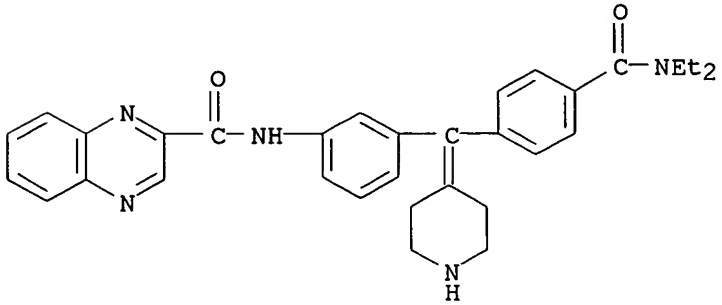
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 141:7139

L23 ANSWER 44 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **692246-95-0** REGISTRY
CN 2-Quinoxalinecarboxamide, N-[3-[[4-[(diethylamino)carbonyl]phenyl]-4-piperidinylidenemethyl]phenyl]-, trifluoroacetate (10:11) (9CI) (CA INDEX NAME)
MF C32 H33 N5 O2 . 11/10 C2 H F3 O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

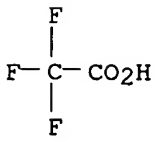
CM 1

CRN 692246-93-8
CMF C32 H33 N5 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

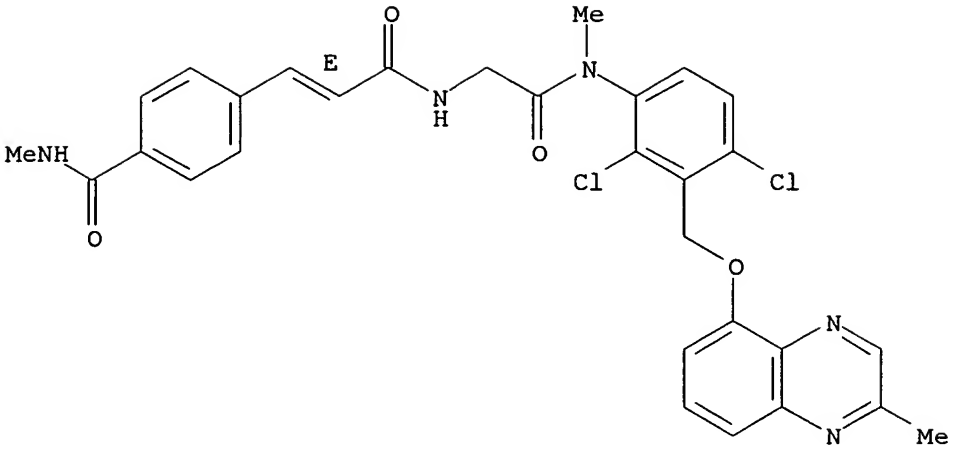


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:423590

L23 ANSWER 45 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **683273-27-0** REGISTRY
CN Benzamide, 4-[(1E)-3-[[2-[[2,4-dichloro-3-[[(2-methyl-5-quinoxalinyl)oxy]methyl]phenyl]methylamino]-2-oxoethyl]amino]-3-oxo-1-propenyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H27 Cl2 N5 O4 . Cl H
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
CRN (215238-13-4)

Double bond geometry as shown.

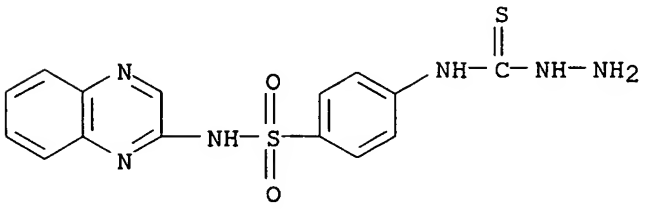


● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:368093

L23 ANSWER 46 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **681235-17-6** REGISTRY
CN Hydrazinecarbothioamide, N-[4-[(2-quinoxalinylamino)sulfonyl]phenyl]-
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H14 N6 O2 S2
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);
RACT (Reactant or reagent)



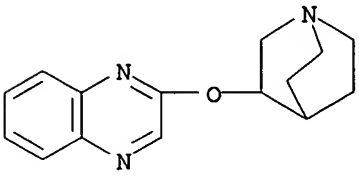
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Searcher : Shears 571-272-2528

REFERENCE 1: 140:357296

L23 ANSWER 48 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **663191-50-2** REGISTRY
CN 1-Azabicyclo[2.2.2]octane, 3-(2-quinoxalinyloxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H17 N3 O
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

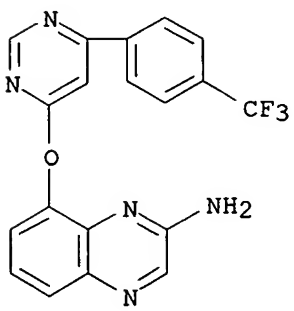


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:199493

L23 ANSWER 49 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **659729-73-4** REGISTRY
CN 2-Quinoxalinamine, 8-[[6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]oxy]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H12 F3 N5 O
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



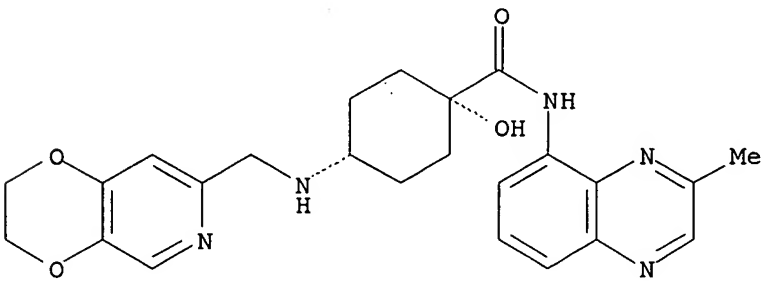
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:181462

L23 ANSWER 52 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **643070-54-6** REGISTRY
CN Cyclohexanecarboxamide, 4-[[(2,3-dihydro-1,4-dioxino[2,3-c]pyridin-7-yl)methyl]amino]-1-hydroxy-N-(3-methyl-5-quinoxalinyl)-, cis- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H27 N5 O4
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

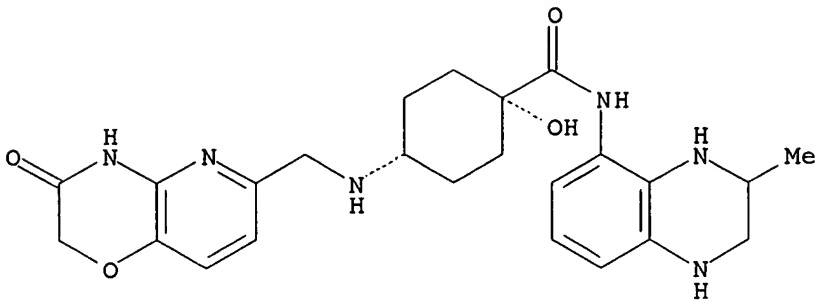
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:94053

L23 ANSWER 55 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **643069-97-0** REGISTRY
CN Cyclohexanecarboxamide, 4-[[(3,4-dihydro-3-oxo-2H-pyrido[3,2-b]-1,4-oxazin-6-yl)methyl]amino]-1-hydroxy-N-(1,2,3,4-tetrahydro-3-methyl-5-quinoxalinyl)-, cis- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H30 N6 O4
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Relative stereochemistry.

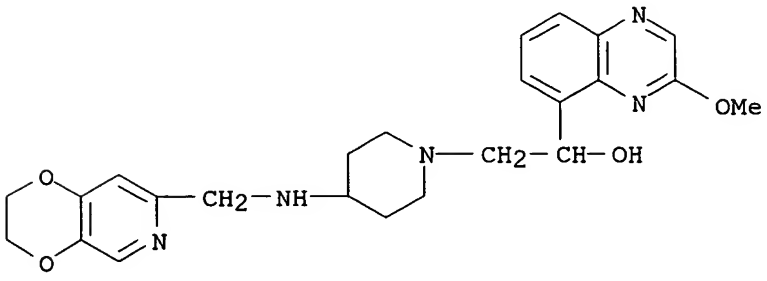


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:94053

L23 ANSWER 58 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **642478-38-4** REGISTRY
CN 5-Quinoxalinemethanol, α-[[4-[[(2,3-dihydro-1,4-dioxino[2,3-c]pyridin-7-yl)methyl]amino]-1-piperidinyl]methyl]-3-methoxy- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H29 N5 O4
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

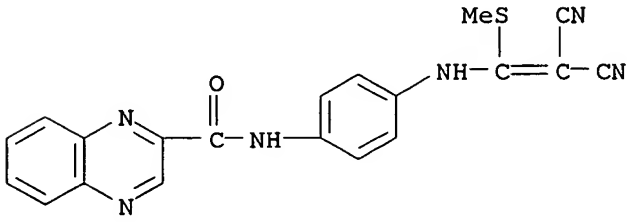


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:94052

L23 ANSWER 59 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **623934-59-8** REGISTRY
CN 2-Quinoxalinecarboxamide, N-[4-[[2,2-dicyano-1-(methylthio)ethenyl]amino]phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H14 N6 O S
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)



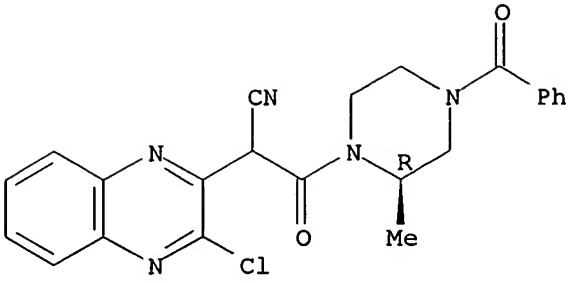
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:381448

L23 ANSWER 61 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **623583-65-3** REGISTRY
CN Piperazine, 4-benzoyl-1-[(3-chloro-2-quinoxalinyl)cyanoacetyl]-2-methyl-, (2R)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H20 Cl N5 O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.

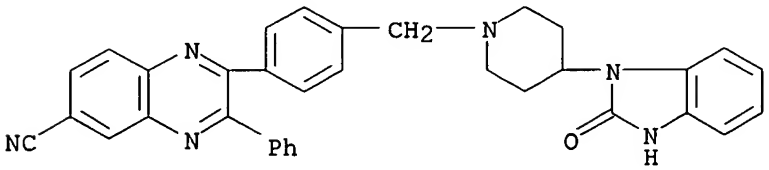


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:381510

L23 ANSWER 62 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **612848-76-7** REGISTRY
CN 6-Quinoxalinecarbonitrile, 2-[4-[[4-(2,3-dihydro-2-oxo-1H-benzimidazol-1-yl)-1-piperidinyl]methyl]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C34 H28 N6 O
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:350754

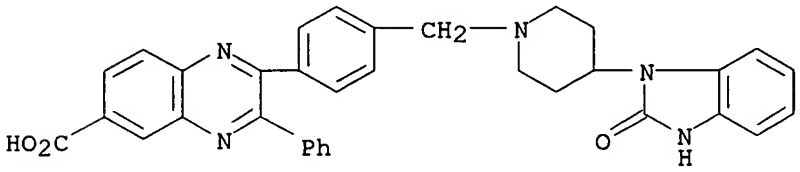
REFERENCE 2: 139:323527

L23 ANSWER 65 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **612847-32-2** REGISTRY
CN 6-Quinoxalinecarboxylic acid, 2-[4-[[4-(2,3-dihydro-2-oxo-1H-benzimidazol-

1-yl)-1-piperidinyl]methyl]phenyl]-3-phenyl-, trifluoroacetate (9CI) (CA INDEX NAME)
MF C34 H29 N5 O3 . x C2 H F3 O2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

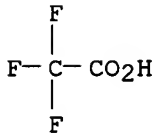
CM 1

CRN 612847-31-1
CMF C34 H29 N5 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

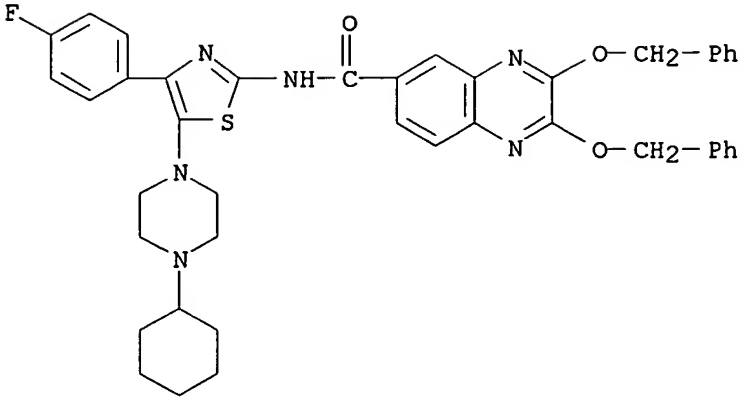
REFERENCE 1: 141:7131

REFERENCE 2: 139:350754

REFERENCE 3: 139:323527

L23 ANSWER 69 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **570405-07-1** REGISTRY
CN 6-Quinoxalinecarboxamide, N-[5-(4-cyclohexyl-1-piperazinyl)-4-(4-fluorophenyl)-2-thiazolyl]-2,3-bis(phenylmethoxy)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C42 H41 F N6 O3 S
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT

(Reactant or reagent); USES (Uses)

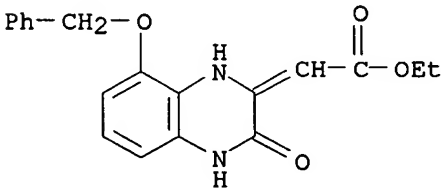


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:149652

L23 ANSWER 70 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **495407-45-9** REGISTRY
CN Acetic acid, [3,4-dihydro-3-oxo-8-(phenylmethoxy)-2(1H)-quinoxalinylidene]-, ethyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Ethyl [8-(benzyloxy)-3-oxo-3,4-dihydroquinoxaline-2(1H)-ylidene]acetate
MF C19 H18 N2 O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

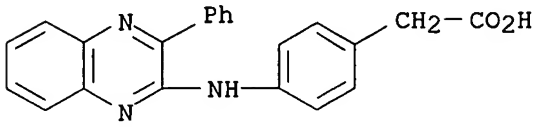


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:153554

L23 ANSWER 73 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **476374-27-3** REGISTRY
CN Benzeneacetic acid, 4-[(3-phenyl-2-quinoxalinyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H17 N3 O2
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

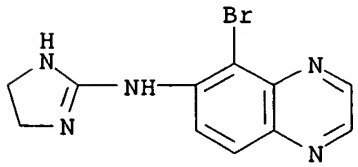
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:83

L23 ANSWER 91 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **474777-33-8** REGISTRY
CN 9,12-Octadecadienoic acid (9Z,12Z)-, compd. with 5-bromo-N-(4,5-dihydro-1H-imidazol-2-yl)-6-quinoxalinamine (1:1) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H32 O2 . C11 H10 Br N5
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

CM 1

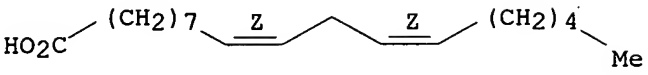
CRN 59803-98-4
CMF C11 H10 Br N5



CM 2

CRN 60-33-3
CMF C18 H32 O2

Double bond geometry as shown.



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

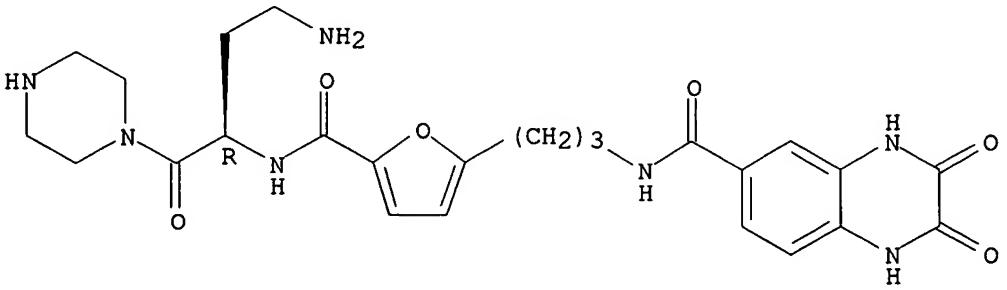
REFERENCE 1: 138:226731

REFERENCE 2: 138:112477

REFERENCE 3: 137:358171

L23 ANSWER 92 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **462119-69-3** REGISTRY
CN 6-Quinoxalinecarboxamide, N-[3-[5-[[[(1R)-3-amino-1-(1-piperazinylcarbonyl)propyl]amino]carbonyl]-2-furanyl]propyl]-1,2,3,4-tetrahydro-2,3-dioxo- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H31 N7 O6
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.

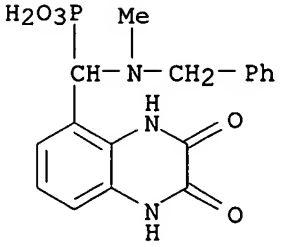


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:257239

L23 ANSWER 97 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **459836-22-7** REGISTRY
CN Phosphonic acid, [[methyl(phenylmethyl)amino](1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxalinyl)methyl]- (9CI) (CA INDEX NAME)
MF C17 H18 N3 O5 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

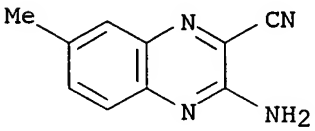


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:226178

L23 ANSWER 104 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **444807-95-8** REGISTRY
CN 2-Quinoxalinecarbonitrile, 3-amino-7-methyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H8 N4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

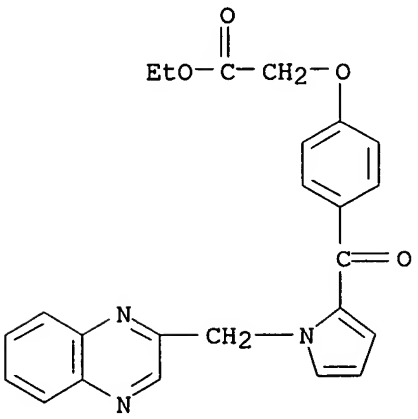
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Searcher : Shears 571-272-2528

REFERENCE 1: 141:133557

REFERENCE 2: 137:134476

L23 ANSWER 105 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **397325-03-0** REGISTRY
CN Acetic acid, [4-[[1-(2-quinoxalinylmethyl)-1H-pyrrol-2-yl]carbonyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-[[2-(4-((Ethoxycarbonyl)methoxy)benzoyl)pyrrol-1-yl]methyl]quinoxaline
MF C24 H21 N3 O4
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

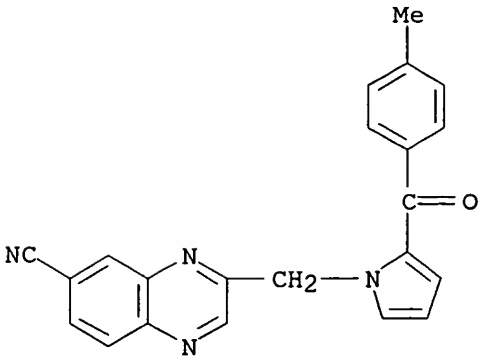
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:159972

REFERENCE 2: 136:167389

L23 ANSWER 107 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **397324-20-8** REGISTRY
CN 6-Quinoxalinecarbonitrile, 3-[[2-(4-methylbenzoyl)-1H-pyrrol-1-yl]methyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 7-Cyano-2-[[2-(4-methylbenzoyl)pyrrol-1-yl]methyl]quinoxaline
FS 3D CONCORD
MF C22 H16 N4 O
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



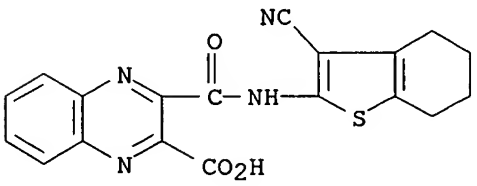
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:159972

REFERENCE 2: 136:167389

L23 ANSWER 111 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **389085-81-8** REGISTRY
CN 2-Quinoxalinecarboxylic acid, 3-[[(3-cyano-4,5,6,7-tetrahydrobenzo[b]thien-2-yl)amino]carbonyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H14 N4 O3 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

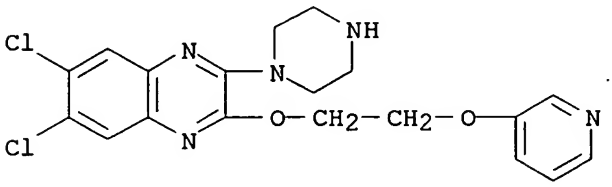


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:102343

L23 ANSWER 114 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **313656-92-7** REGISTRY
CN Quinoxaline, 6,7-dichloro-2-(1-piperazinyl)-3-[2-(3-pyridinyloxy)ethoxy]-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-[2-(3-Pyridinyloxy)ethoxy]-3-(1-piperazinyl)-6,7-dichloroquinoxaline
FS 3D CONCORD
MF C19 H19 Cl2 N5 O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



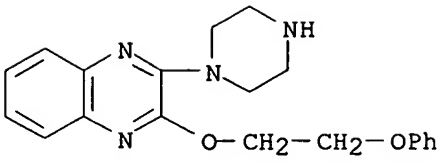
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:294982

REFERENCE 2: 134:56689

L23 ANSWER 116 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **313654-02-3** REGISTRY
CN Quinoxaline, 2-(2-phenoxyethoxy)-3-(1-piperazinyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-(2-Phenoxyethoxy)-3-(1-piperazinyl)quinoxaline
FS 3D CONCORD
MF C20 H22 N4 O2
CI COM
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



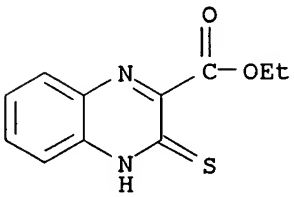
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:294982

REFERENCE 2: 134:56689

L23 ANSWER 117 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **278186-19-9** REGISTRY
CN 2-Quinoxalinecarboxylic acid, 3,4-dihydro-3-thioxo-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H10 N2 O2 S
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:78924

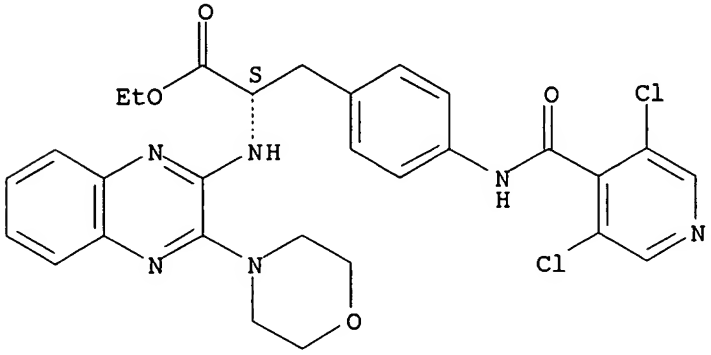
REFERENCE 2: 136:263138

REFERENCE 3: 133:58781

L23 ANSWER 118 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **263275-11-2** REGISTRY
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[3-(4-

morpholinyl)-2-quinoxalinyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H28 Cl2 N6 O4
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

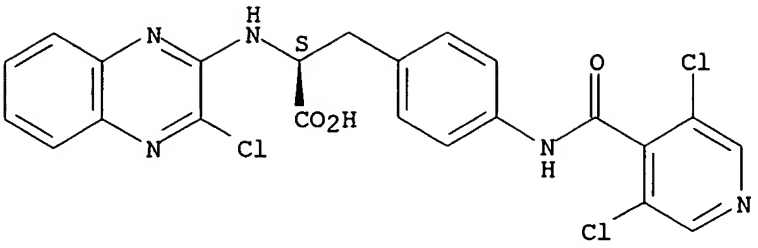
REFERENCE 1: 136:135022

REFERENCE 2: 136:135019

REFERENCE 3: 132:265501

L23 ANSWER 119 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **263275-09-8** REGISTRY
CN L-Phenylalanine, N-(3-chloro-2-quinoxalinyl)-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H16 Cl3 N5 O3
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

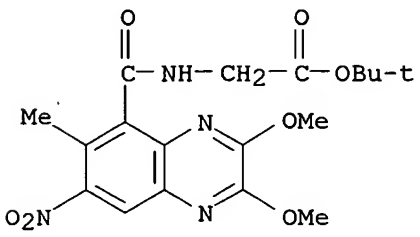
3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:135022

REFERENCE 2: 136:135019

REFERENCE 3: 132:265501

L23 ANSWER 120 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **258508-93-9** REGISTRY
CN Glycine, N-[(2,3-dimethoxy-6-methyl-7-nitro-5-quinoxalinyl)carbonyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)
OTHER NAMES:
CN [(2,3-Dimethoxy-6-methyl-7-nitroquinoxaline-5-carbonyl)amino]acetic acid tert-butyl ester
FS 3D CONCORD
MF C18 H22 N4 O7
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: PREP (Preparation)



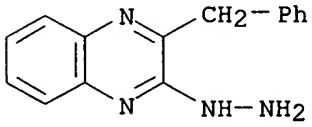
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:118473

REFERENCE 2: 132:166212

L23 ANSWER 121 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **223929-23-5** REGISTRY
CN 2(1H)-Quinoxalinone, 3-(phenylmethyl)-, hydrazone (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (3-Benzylquinoxalin-2-yl)hydrazine
FS 3D CONCORD
MF C15 H14 N4
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

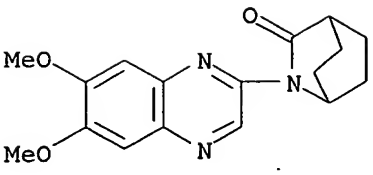
REFERENCE 1: 141:314272

REFERENCE 2: 139:36744

REFERENCE 3: 132:237060

REFERENCE 4: 130:325156

L23 ANSWER 122 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **217093-53-3** REGISTRY
CN 2-Azabicyclo[2.2.2]octan-3-one, 2-(6,7-dimethoxy-2-quinoxalinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H19 N3 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:285655

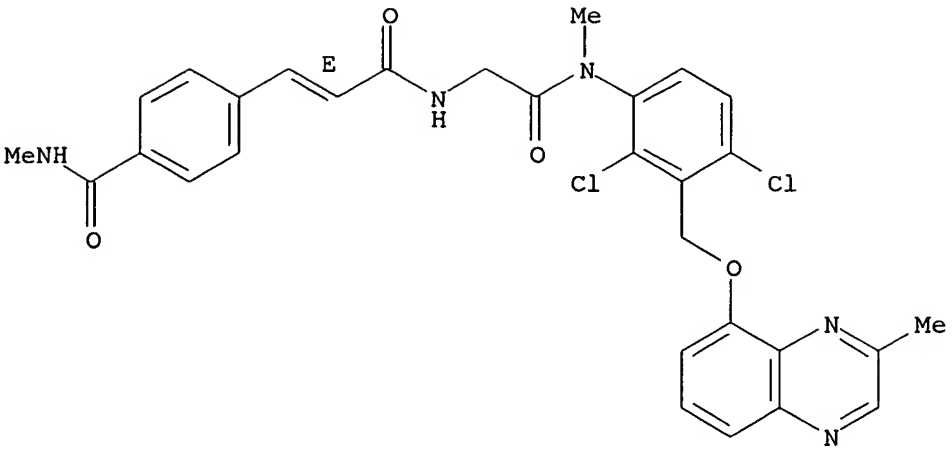
REFERENCE 2: 134:131553

REFERENCE 3: 133:17479

REFERENCE 4: 130:52435

L23 ANSWER 123 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **215238-12-3** REGISTRY
CN Benzamide, 4-[(1E)-3-[[2-[[2,4-dichloro-3-[[(3-methyl-5-quinoxalinyl)oxy]methyl]phenyl]methylamino]-2-oxoethyl]amino]-3-oxo-1-propenyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H27 Cl2 N5 O4 . Cl H
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
CRN (215238-10-1)

Double bond geometry as shown.



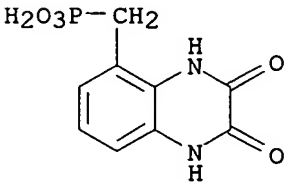
● HCl

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:368093

REFERENCE 2: 129:325738

L23 ANSWER 124 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **187479-26-1** REGISTRY
CN Phosphonic acid, [(1,2,3,4-tetrahydro-2,3-dioxo-5-quinoxalinyl)methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H9 N2 O5 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

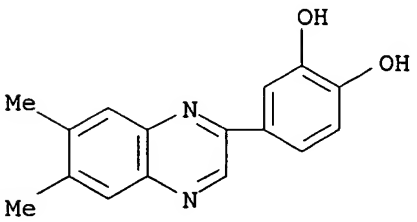
Searcher : Shears 571-272-2528

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:226178

REFERENCE 2: 126:186210

L23 ANSWER 126 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **168835-90-3** REGISTRY
CN 1,2-Benzenediol, 4-(6,7-dimethyl-2-quinoxalinyl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN AG 1433
CN SU 1433
FS 3D CONCORD
DR 197592-59-9
MF C16 H14 N2 O2
CI COM
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, CHEMCATS, IMSDRUGNEWS, IMSRESEARCH, TOXCENTER, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1907 TO DATE)
14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:270356

REFERENCE 2: 139:122710

REFERENCE 3: 139:106450

REFERENCE 4: 138:8422

REFERENCE 5: 136:53764

REFERENCE 6: 131:346563

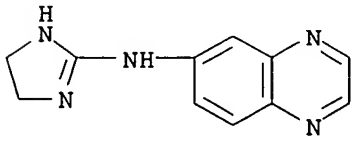
REFERENCE 7: 131:322425

REFERENCE 8: 129:175652

REFERENCE 9: 129:54393

REFERENCE 10: 128:154102

L23 ANSWER 127 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **91147-43-2** REGISTRY
CN 6-Quinoxalinamine, N-(4,5-dihydro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN UK 41511
FS 3D CONCORD
MF C11 H11 N5
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

14 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:265771

REFERENCE 2: 138:226731

REFERENCE 3: 138:112477

REFERENCE 4: 137:358171

REFERENCE 5: 136:123675

REFERENCE 6: 136:6009

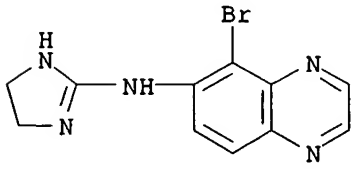
REFERENCE 7: 134:188222

REFERENCE 8: 133:89544

REFERENCE 9: 123:329809

REFERENCE 10: 123:217719

L23 ANSWER 128 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **59803-98-4** REGISTRY
CN 6-Quinoxalinamine, 5-bromo-N-(4,5-dihydro-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 5-Bromo-6-(2-imidazolin-2-ylamino)quinoxaline
CN AGN 190342
CN Brimonidine
CN Bromoxidine
CN UK 14304
CN UK 14304-18
FS 3D CONCORD
DR 109826-55-3
MF C11 H10 Br N5
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CBNB, CHEMCATS, CIN, CSCHEM, DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK*, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: WHO
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PROC (Process); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

719 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
721 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:86673

REFERENCE 2: 142:69446

REFERENCE 3: 142:62657

REFERENCE 4: 142:49146

REFERENCE 5: 142:775

REFERENCE 6: 141:384335

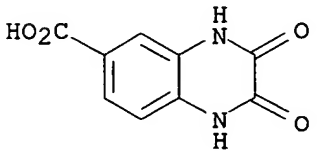
REFERENCE 7: 141:361003

REFERENCE 8: 141:355430

REFERENCE 9: 141:355374

REFERENCE 10: 141:301455

L23 ANSWER 129 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **14121-55-2** REGISTRY
CN 6-Quinoxalinecarboxylic acid, 1,2,3,4-tetrahydro-2,3-dioxo- (7CI, 9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 6-Quinoxalinecarboxylic acid, 2,3-dihydroxy- (8CI)
OTHER NAMES:
CN 2,3-Dihydroxy-6-quinoxalinecarboxylic acid
CN NSC 211121
FS 3D CONCORD
MF C9 H6 N2 O4
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

17 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

Searcher : Shears 571-272-2528

17 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 139:240337

REFERENCE 2: 137:257239

REFERENCE 3: 136:210595

REFERENCE 4: 136:151182

REFERENCE 5: 133:4414

REFERENCE 6: 131:74941

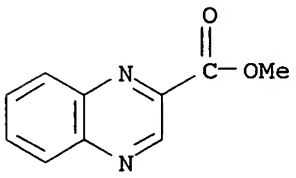
REFERENCE 7: 122:108650

REFERENCE 8: 122:10070

REFERENCE 9: 118:182828

REFERENCE 10: 101:7194

L23 ANSWER 130 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **1865-11-8** REGISTRY
CN 2-Quinoxalinecarboxylic acid, methyl ester (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H8 N2 O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, TOXCENTER
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation); RACT (Reactant or reagent); NORL (No role in record)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 142:93713

REFERENCE 2: 138:73233

REFERENCE 3: 136:274953

REFERENCE 4: 108:112059

REFERENCE 5: 94:208098

REFERENCE 6: 62:29499

REFERENCE 7: 54:133474

REFERENCE 8: 54:133473

REFERENCE 9: 54:133472

L23 ANSWER 131 OF 131 REGISTRY COPYRIGHT 2005 ACS on STN
RN **91-19-0** REGISTRY
CN Quinoxaline (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1,4-Benzodiazine
CN 1,4-Diazanaphthalene
CN 1,4-Naphthyridine
CN Benzoparadiazine
CN Benzopyrazine
CN Benzo[a]pyrazine
CN Phenopiazine
CN Phenpiazine
CN Quinazine
FS 3D CONCORD
MF C8 H6 N2
CI COM, RPS
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DETHERM*, EMBASE, GMELIN*, HODOC*, IFICDB, IFIPAT, IFIUDB, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TULSA, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Preprint; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); CMBI (Combinatorial study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
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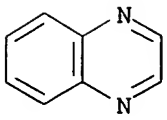
PRP (Properties); RACT (Reactant or reagent); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1875 REFERENCES IN FILE CA (1907 TO DATE)
579 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1878 REFERENCES IN FILE CAPLUS (1907 TO DATE)
22 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 142:120589

REFERENCE 2: 142:114039

REFERENCE 3: 142:113926

REFERENCE 4: 142:102844

REFERENCE 5: 142:93707

REFERENCE 6: 141:418065

REFERENCE 7: 141:416008

REFERENCE 8: 141:403674

REFERENCE 9: 141:366582

REFERENCE 10: 141:366136

FILE 'CAOLD' ENTERED AT 09:59:39 ON 07 FEB 2005
L24 26 S L23

L24 ANSWER 1 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:20778a CAOLD
TI microbiocidal compns. derived from quinoxaline
AU Hattori, Junnosuke; Koike, S.; Ozaki, T.; Yoshioka, H.; Sugiyama, H.
DT Patent
TI quinoxaline, microbiocidal compns. derived from
PA Sumitomo Chemical Co., Ltd.
DT Patent

PATENT NO.	KIND	DATE
GB 1043042		

IT **91-19-0** 2075-99-2 2347-47-9 13313-95-6

L24 ANSWER 2 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:16097f CAOLD
TI thin-layer chromatography of azines and of aromatic N heterocycles on

Al2O3
AU Klemm, LeRoy H.; Klopfenstein, C. E.; Kelly, H. P.
IT 85-02-9 **91-19-0** 91-62-3 91-63-4 92-82-0
103-30-0 119-65-3 119-91-5 207-11-4 215-64-5 217-68-5
225-02-5 225-06-9 225-51-4 229-87-8 230-17-1 230-27-3
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260-94-6 272-67-3 366-18-7 484-11-7 491-35-0 538-49-8
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14722-38-4 89939-13-9 92552-20-0

L24 ANSWER 3 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:13186h CAOLD
TI transition-metal quinoxaline complexes - (III) Cu(II) derivs. with substituted quinoxalines
AU Billing, D. E.; Underhill, A. E.; Adams, D. M.; Morris, D. M.
IT **91-19-0** 1684-14-6 2379-55-7 7251-61-8 14284-58-3
14376-51-3 26316-88-1 26316-89-2 36005-76-2 94006-95-8 94502-35-9
101546-44-5 101546-46-7

L24 ANSWER 4 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:7307a CAOLD
TI polymerization of acetylenic hydrocarbons
AU Dubeck, Michael; Filbey, A. H.
PA Ethyl Corp.
DT Patent

PATENT NO.	KIND	DATE
US 3256260		1966

IT **91-19-0** 92-82-0 107-19-7 229-87-8 230-07-9
253-52-1 253-66-7 253-82-7 288-13-1 288-32-4 288-36-8
289-80-5 289-96-3 290-37-9 290-38-0 471-25-0 557-12-0
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15625-54-4 15793-12-1 31811-17-3 52445-55-3

L24 ANSWER 5 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:7004b CAOLD
TI radical phenylation of bicyclic heterocyclic compds.
AU Dou, Henri J. M.; Lynch, B. M.
IT **91-19-0** 95-16-9 1632-83-3

L24 ANSWER 6 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA65:2646a CAOLD
TI nitrogenous heterocycles in cigaret smoke condensate
AU Testa, Albert; Testa, P.
IT **91-19-0** 290-37-9

L24 ANSWER 7 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:18711c CAOLD

TI far-ultraviolet spectra of azines in solution
AU Favini, Giorgio; Bellobono, I. R.
IT **91-19-0** 253-52-1 253-66-7 253-82-7 289-80-5
290-37-9 290-87-9

L24 ANSWER 8 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10625e CAOLD
TI 14N hyperfine structure in electron spin resonance spectra of heterocyclic anions
AU Henning, J. C. M.
IT **91-19-0** 92-82-0 254-79-5 289-80-5 290-37-9
6918-15-6 89939-13-9

L24 ANSWER 9 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10608e CAOLD
TI measurement of the polarization of the phosphorescence of certain diazines in vitreous solution at 77°K. and interpretation of the results by spin-orbit interaction
AU Loustauneau, Pierre
IT **91-19-0** 290-37-9

L24 ANSWER 10 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10600g CAOLD
TI singlet-singlet and triplet-triplet absorption spectra of certain diazines in crystallized solns.
AU Loustauneau, Pierre; Nouchi, G.
IT **91-19-0** 92-82-0

L24 ANSWER 11 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:10547b CAOLD
TI magnetophotoselection of the lowest excited triplet state of aromatic mols.
AU El-Sayed, Mostafa A.; Siegel, S.
IT **91-19-0** 538-04-5 1146-65-2 1517-22-2

L24 ANSWER 12 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:9574d CAOLD
TI inductive and mesomeric effects in substituted organic mols. - (XX) pyrazine derivs.
AU Lumbroso, Henri; Palamidessi, G.
IT **91-19-0** 1628-89-3

L24 ANSWER 13 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:9117c CAOLD
TI heterogeneous catalysis by organic conjugated polymers-electron spin resonance and structural factors
AU Gallard-Nechtschein, Jacqueline; Laederich, T.; Nechtschein, M.; Pecher, A.; Salle, R.; Traynard, P.
IT 51-17-2 **91-19-0** 32518-77-7

L24 ANSWER 14 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:9073c CAOLD
TI azanaphthalenes - (I) Hueckel orbital calcns.
AU Wait, Samuel C., Jr.; Wesley, J. W.
IT 91-18-9 **91-19-0** 253-45-2 253-50-9 253-52-1
253-61-2 253-66-7 253-69-0 253-72-5 253-74-7 253-82-7

253-83-8 253-86-1 253-87-2 253-88-3 254-60-4 254-61-5
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6133-97-7 6133-98-8 6133-99-9 6380-84-3 7666-88-8 89939-13-9

L24 ANSWER 15 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA64:7535h CAOLD
TI infrared spectra of some diaza- and triazanaphthalenes and of 1,4,5,8-tetraazanaphthalene
AU Armarego, W. L. F.; Barlin, G. B.; Spinner, E.
DT Patent
IT **91-19-0** 253-82-7 254-79-5 255-53-8 14336-94-8
14380-59-7

L24 ANSWER 16 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:17326g CAOLD
TI calcn. of electronic spectra of azabenzenes and azanaphthalenes by the Pariser-Parr-Pople method
AU Favini, Giorgio; Vandoni, I.; Simonetta, M.
IT 91-18-9 **91-19-0** 253-45-2 253-52-1 253-66-7
253-69-0 253-72-5 253-82-7 253-86-1 253-87-2 254-60-4
254-61-5 254-79-5 254-80-8 254-86-4 254-87-5 255-53-8
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322-46-3 592-59-6 89939-13-9

L24 ANSWER 17 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:10883b CAOLD
TI analysis of the proton nuclear magnetic resonance spectra of heteroaromatic systems - (V) diazanaphthalenes
AU Black, Peter J.; Heffernan, M. L.
IT **91-19-0** 253-52-1 253-66-7 253-82-7

L24 ANSWER 18 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:1353d CAOLD
TI spectroscopy and photosensitization of various photochromic spiropyrans
AU Becker, Ralph S.; Roy, J. K.
IT **91-19-0** 1485-92-3 1498-88-0 1498-89-1 1592-43-4

L24 ANSWER 19 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:168c CAOLD
TI shifts and electron ds. in N heterocyclic mols.
AU Gawer, Albert; Dailey, B. P.
IT **91-19-0** 253-52-1 253-66-7 253-82-7 254-79-5
289-80-5 290-37-9 12015-14-4 89939-13-9

L24 ANSWER 20 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA63:36b CAOLD
TI zero-field splittings - (V) aromatic N heterocycles
AU Boorstein, Seth A.; Gouterman, M.
IT **91-19-0** 290-37-9

L24 ANSWER 21 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA62:14062c CAOLD
TI luminescence and the triplet state
AU Rousset, Auguste
IT **91-19-0** 92-82-0 290-37-9

L24 ANSWER 22 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA62:11833f CAOLD
TI nitrofuran derivs. having a triazine ring
AU Kodama, Yutaka; Takai, A.; Saikawa, I.; Haseda, M.
PA Toyama Chemical Industry Co., Ltd.
DT Patent

PATENT NO.	KIND	DATE
JP 64028256		1964

IT 842-81-9 893-25-4 893-26-5 895-65-8 900-70-9 952-11-4
14121-55-2

L24 ANSWER 23 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA62:8525f CAOLD
TI calcn. of electronic spectra of azabenzenes and azanaphthalenes by the Pariser-Parr-Pople method
AU Favini, Giorgio; Vandoni, I.; Simonetta, M.
IT 91-18-9 **91-19-0** 253-45-2 253-50-9 253-52-1
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290-87-9 290-96-0 322-46-3 592-59-6 89939-13-9

L24 ANSWER 24 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA62:5215c CAOLD
TI basic cleavages of arylsulfonamides
AU Negishi, Eiichi; Day, A. R.
IT 1096-43-1 1865-09-4 1865-10-7 **1865-11-8** 1865-12-9
1865-13-0 1865-14-1 1865-15-2 1865-16-3 1865-18-5 1865-19-6
2101-20-4 2101-21-5 2680-41-3 2762-31-4 3442-30-6 3442-50-0
3753-91-1 4092-09-5 4099-43-8 63068-63-3 105042-90-8

L24 ANSWER 25 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA54:25560a CAOLD
TI antibiotics from Streptomyces
AU Prelog, Vladimir; Gaeumann, E.; Wettstein, A.
DT Patent
TI proteolytic enzyme
PA American Cyanamid Co.
DT Patent

PATENT NO.	KIND	DATE
DE 1025572		

IT 879-65-2 **1865-11-8**

L24 ANSWER 26 OF 26 CAOLD COPYRIGHT 2005 ACS on STN
AN CA52:6361h CAOLD
TI phenazines - (XV) ring cleavage of phenazine(1) 2,3-quinoxalinediacarboxylic acid

AU Yoshioka, Ichiro; Otomasu, H.
IT **1865-11-8** 2876-17-7 2876-18-8 5182-90-1 5660-34-4
6924-99-8 54571-06-1 110490-03-4

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L26 0 SEA ABB=ON PLU=ON L23(L)(PHARM? OR DRUG OR PRODRUG OR MEDICIN## OR MEDICAT?)

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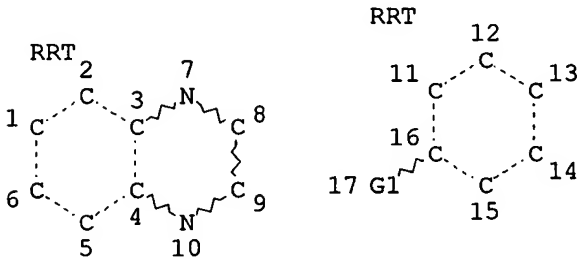

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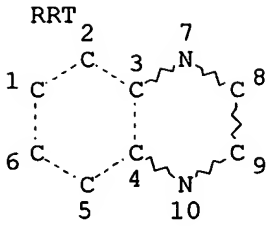
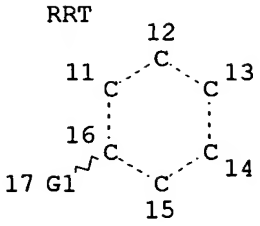
CONNECT IS X2 RC AT 10
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L48 276 SEA FILE=CASREACT SSS FUL L46 (2173 REACTIONS)
L53 STR





PRO

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18 19 20 21 22

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VAR G2=O/S/N
VAR G3=C/S
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CONNECT IS X2 RC AT 10
DEFAULT MLEVEL IS ATOM
GGCAT IS PCY UNS AT 18
GGCAT IS UNS AT 20
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E2 N AT 18

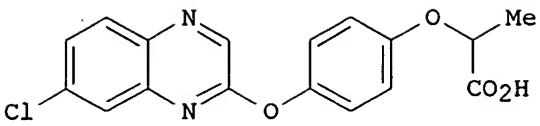
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE
L54 1 SEA FILE=CASREACT SUB=L48 SSS FUL L53 (5 REACTIONS)

100.0% DONE 2169 VERIFIED 5 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

L54 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 135:76849 CASREACT
TITLE: Design, Synthesis, and Biological Evaluation of Analogues of the Antitumor Agent, 2-{4-[(7-Chloro-2-quinoxalinyl)oxy]phenoxy}propionic Acid (XK469)
AUTHOR(S): Hazeldine, Stuart T.; Polin, Lisa; Kushner, Juiwanna; Paluch, Jennifer; White, Kathryn; Edelstein, Matthew; Palomino, Eduardo; Corbett, Thomas H.; Horwitz, Jerome P.
CORPORATE SOURCE: Department of Internal Medicine Division of Hematology and Oncology, Wayne State University School of Medicine, Detroit, MI, 48201, USA
SOURCE: Journal of Medicinal Chemistry (2001), 44(11), 1758-1776
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

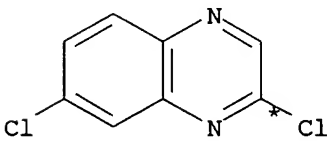
Searcher : Shears 571-272-2528



I

AB 2-{4-[(7-Chloro-2-quinoxalinyl)oxy]phenoxy}propionic acid (XK469) I is among the most highly and broadly active antitumor agents to have been evaluated and scheduled to enter clin. trials in 2001. The mechanism or mechanisms of action of I remain to be elaborated. Accordingly, an effort was initiated to establish a pharmacophore hypothesis to delineate the requirements of the active site, via a comprehensive program of synthesis of analogs of I and evaluation of the effects of structural modification(s) on solid tumor activity. The strategy formulated chose to dissect the two-dimensional parent structure into three regions: I, ring A of quinoxaline; II, the hydroquinone connector linkage; and III, the lactic acid moiety-to determine the resultant in vitro and in vivo effects of chemical alterations in each region. Neither the A-ring unsubstituted nor the B-ring 3-chloro-regioisomer of I showed antitumor activity. The modulating antitumor effect(s) of substituents of differing electronegativities, located at the several sites comprising the A-ring of region I, were next ascertained. Thus, a halogen substituent, located at the 7-position of a 2-{4-[(2-quinoxalinyl)oxy]phenoxy}propionic acid, generated the most highly and broadly active antitumor agents. A Me, methoxy, or an azido substituent at this site generated a much less active structure, whereas 5-, 6-, 8-chloro-, 6-, 7-nitro, and 7-amino derivs. all proved to be essentially inactive. When the connector linkage (region II) of I was changed from that of a hydroquinone to either a resorcinol or a catechol derivative, all antitumor activity was lost. Of the carboxylic acid derivs. of I (region III), i.e., CONH2, CONHMe, CONMe2, CONHOH, CONHNH2, CN, or CN4H (tetrazole), only the monomethyl- and N,N-dimethylamides proved to be active.

RX(61) OF 233 ...**Z** + **DI** ===> **DO**...



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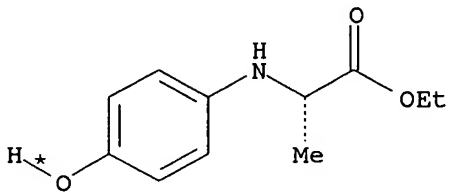

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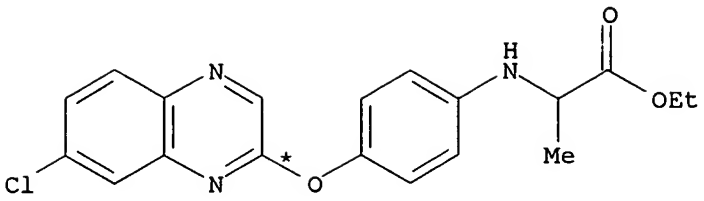

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YIELD 84%

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RGT BL 584-08-7 K2CO3
PRO DO **347162-61-2**
SOL 75-05-8 MeCN
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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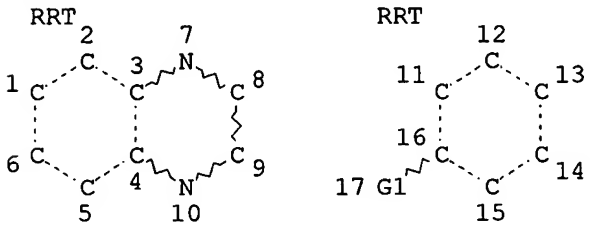
L51 STR



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VAR G2=O/S/N
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DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L55 14 SEA L51

L55 ANSWER 1 OF 14 DJSMDS COPYRIGHT 2005 THE THOMSON CORP on STN
AN 1999:1059 DJSMDS
TI 2-ARYLOXY- FROM 2-CHLORO-QUINOXALINES AND PHENOLS
AU Cuenca, A.
SO Synth Commun, 29(8), p.1393-9 (1999)

CODEN: SYNCAV ISSN: 0039-7911
DT Journal
VI 25-5
AB Cf. 1987:76525C. The method is simple, mild and starting materials are accessible. Higher temperatures and longer reaction times are required for the reaction to proceed in the absence of silver nitrate. Cf. 1998:1052. For further examples, (74-83%), see citation 1.

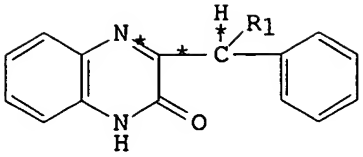
RX(1) OF 1 **A** + **B** ===> **C**

A B C
YIELD 86.0%

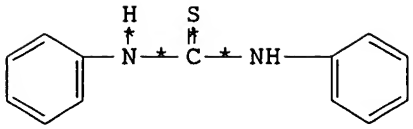
RX(1) RCT A, **13976**
B, **5784**; 1 Eq.
SOL 23, DMF
CAT 879, AgNO3; 10 mol.%
135, KOH; 1 Eq.
PRO C, **103447**
T 68.0 Cel
TIM 1.0 hr
CMT Path A

L55 ANSWER 2 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200446155 CHEMINFORMRX
TI Fused Polycyclic Nitrogen-Containing Heterocycles. Part 7. Reaction Products of 3-(α-Chlorobenzyl)-1,2-dihydroquinoxalin-2-one and Thioureas as Key Intermediate Compounds in the Synthesis of Thiazolo[3,4-a]quinoxalines.
AU KALININ, A. A.; MAMEDOV, V. A.; RIZVANOV, I. K.; LEVIN, Y. A.
CS Arbuzov Inst. Org. Phys. Chem., Kazan Res. Cent., Russ. Acad. Sci., Kazan' 420088, Russia
SO Russ. J. Org. Chem., 40(4), 527-533 (2004)
CODEN: RJOCEQ ISSN: 1070-4280
LA English
AB Quinoxalinone derivative (I) is subjected to reactions with reagents which are equivalents of the NCS species, in particular with (II), (V), 2-sulfanylbenzimidazole, and 2-sulfanylbenzothiazole. Attempted intramolecular cyclization reactions of the latter compounds fail. Heating thiourea (II) or N,N'-diphenylthiourea (VI) with quinoxalinone (I) in dioxane with subsequent addition of acetic anhydride affords the thiazoloquinoxalines (IV) and (VII). Unfortunately, the yield of (IV) for this one-pot procedure is considerably lower than in the two-step synthesis via isothioureide (V). Also, structures containing no heterocyclic system can be regarded as precursors of the title compounds. For example, synthetic equivalents for the required synthons are chloropyruvate (VIII), potassium thiocyanate (IX), and o-phenylenediamine (X).

RX(4) OF 6 A + I ===> J

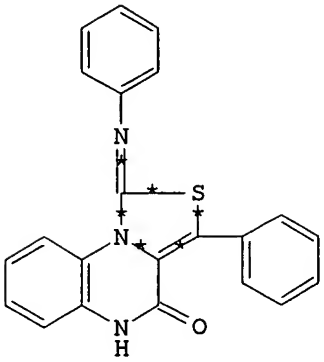


I



VI

(4) →



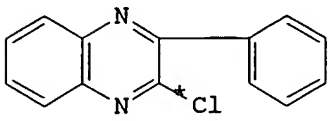
VII
YIELD 10.0%

RX(4) RCT I, **764252**
VI, **34607** (102-08-9)
STAGE(1)
SOL 80 (123-91-1), dioxane
T.KW REFLUX
STAGE(2)
RGT 4 (108-24-7), Ac2O
3 (64-19-7), AcOH
T.KW REFLUX
PRO VII, **507274**
YDS 10.0 %
KW addition; alkylation; N-alkylation; S-alkylation
NTE reaction:I 1.(VI) -> VII

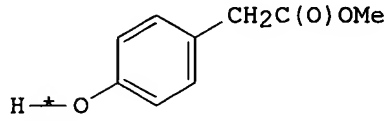
L55 ANSWER 3 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200427140 CHEMINFORMRX
TI Quinoxaline Chemistry. Part 17. Methyl [4-(Substituted-2-quinoxalinyloxy)phenyl]acetates and Ethyl N-{[4-(Substituted-2-quinoxalinyloxy)phenyl]acetyl}glutamates Analogues of Methotrexate:

Synthesis and Evaluation of in vitro Anticancer Activity.
AU PIRAS, S.; LORIGA, M.; PAGLIETTI, G.
CS Dip. Farm. Chim. Tossicol., Univ. Sassari, I-07100 Sassari, Italy
SO Farmaco, 59(3), 185-194 (2004)
CODEN: FRMCE8 ISSN: 0014-827X
LA English
AB Compounds (VII) and (VIb) show the strongest anticancer activity of all tested compounds.

RX(1) OF 18 A + B ===> C...

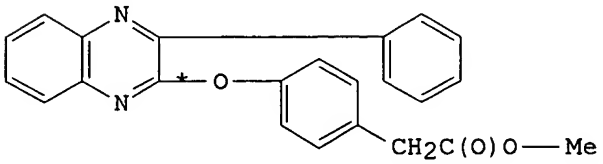


I



II

(1) →

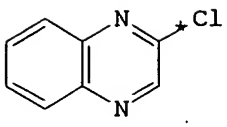


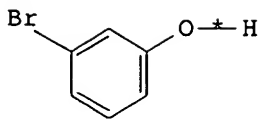
III
YIELD 90.0%

RX(1) RCT I, **391494**
II, **468959** (14199-15-6)
RGT 1042 (534-17-8), Cs2CO3
SOL 76 (68-12-2), DMF
PRO III, **1021305**
YDS 90.0 %
T 70.0 Cel
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III, example: 1

L55 ANSWER 4 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200231171 CHEMINFORMRX
TI Silver(I)-Catalyzed Synthesis of Novel Quinoxaline Derivatives.
AU RIZZO, A.; CAMPOS, G.; ALVAREZ, A.; CUENCA, A.
CS Dep. Quim., Univ. Simon Bolivar, Caracas 1080-A, Venez.
SO Synth. Commun., 32(5), 813-817 (2002)
CODEN: SYNCAV ISSN: 0039-7911
LA English
AB The reaction of chloroquinoxaline (I) with phenoxide ion derivatives (II) utilizing Ag+ as catalyst provides an excellent method for the preparation of the title compounds (III).

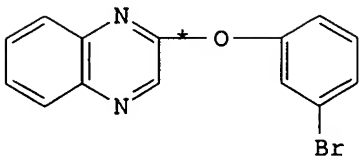
RX(1) OF 4 A + B ===> C





I II

(1)

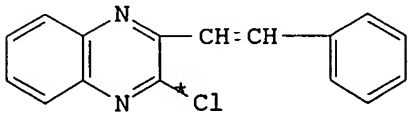


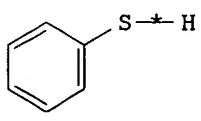
III
YIELD 68.0%

RX(1) RCT I, **157891** (1448-87-9)
II, **22002** (591-20-8)
RGT 1160 (1310-58-3), KOH
SOL 76 (68-12-2), DMF
CAT 1177 (7761-88-8), AgNO3
PRO III, **890723**
YDS 68.0 %
T 70.0 - 81.0 Cel
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III, example: 1

L55 ANSWER 5 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200140147 CHEMINFORMRX
TI Studies on the Synthesis of 2-Phenylsulfonyl-3-styrylquinoxalines.
AU KRISHNAN, V. S. H.; CHOWDARY, K. S.; DUBEY, P. K.; VIJAYA, S.
CS Dep. Chem., Coll. Eng., JNT Univ., Kukatpally 500 072, India
SO Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem., 40(7), 565-573 (2001)
CODEN: IJSBDB ISSN: 0376-4699
LA English
AB Several variations of a synthetic pathway to the title compounds (VII) starting from 3-methylbenzo-1H-dihydropyrazine-2-one (I) are described.

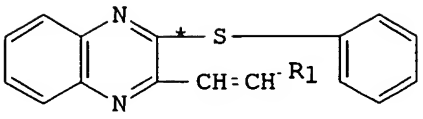
RX(9) OF 52 ...K + Q ===> R...

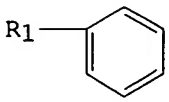




IV V

(9)



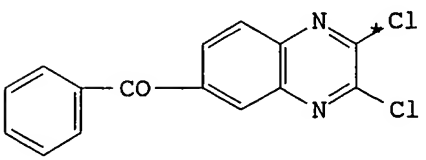


VI
YIELD 95.0%

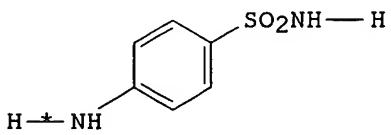
RX(9) RCT IV, **834480**
V, **211** (108-98-5)
RGT 216 (121-44-8), Et3N
SOL 123 (67-56-1), MeOH
PRO VI, **834484**
YDS 95.0 %
T.KW REFLUX
KW arylation
NTE reaction:IV (V) -> VI, example: 1

L55 ANSWER 6 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200126156 CHEMINFORMRX
TI Some Nucleophilic Reactions with 6-Benzoyl-2,3-dichloroquinoxaline: Synthesis of Tetrazolo[1,5-a]quinoxaline, 2-Methylidene-1,3-dithiolo[4,5-b]quinoxalines, Quinoxalino[2,3-b]quinoxalines and Pyrazolo[1',5':1,2]imidazolo[4,5-b]quinoxalines.
AU EL-GABY, M. S. A.; EL-SHARIEF, A. M. S.; AMMAR, Y. A.; MOHAMED, Y. A.; EL-SALAM, A. A. A.
CS Dep. Chem., Fac. Sci., Al-Azhar Univ., Assuit 71524, Egypt
SO Indian J. Chem., Sect. B: Org. Chem. Incl. Med. Chem., 40(3), 195-200 (2001)
CODEN: IJSBDB ISSN: 0376-4699
LA English
AB The starting compound (I) is subjected to some nucleophilic reagents to study the effect of the benzoyl group on the reactivity of the two chlorine atoms.

RX(2) OF 11 A + E ===> F

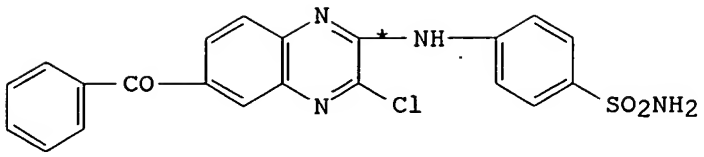


I



II

(2) →

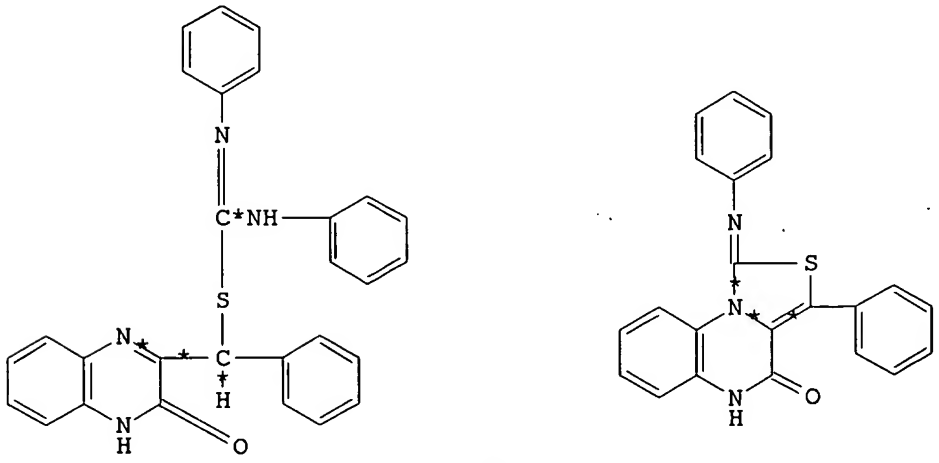


III
YIELD 60.0%

RX(2) RCT I, **85308** (143702-67-4)
II, **19559** (63-74-1)
SOL 76 (68-12-2), DMF
PRO III, **814530**
YDS 60.0 %
T.KW REFLUX
KW arylation
NTE reaction:I (II) -> III, example: 2

L55 ANSWER 7 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 200037168 CHEMINFORMRX
TI 3-Aryl-1-imino-4-oxo-4,5-dihydrothiazolo[3,4-a]quinoxalines. Retrosynthetic Approach.
AU MAMEDOV, V. A.; KALININ, A. A.; GUBAIDULLIN, A. T.; NURKHAMETOVA, I. Z.; LITVINOV, I. A.; LEVIN, Y. A.
CS Arbuzov Inst. Org. Phys. Chem., Kazan Sci. Cent., Russ. Acad. Sci., Kazan 420088, Russia
SO Chem. Heterocycl. Compd. (N. Y.), 35(12), 1459-1473 (1999)
CODEN: CHCCAL ISSN: 0009-3122
LA English
AB Methods for constructing fused thiazoloquinoxaline systems such as (IV) and (VII) from 3-(α-chlorobenzyl)quinoxalinones (I) via the intermediacy of corresponding 3-(α-thiocyanatobenzyl)- and 3-(α-isothioureidobenzyl) derivatives are developed.

RX(6) OF 9 ...K ===> L

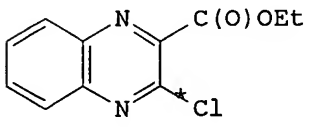


VI (6) VII
YIELD 33.0%

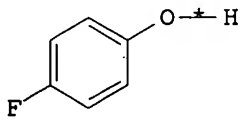
RX(6) RCT VI, **764257**
SOL 3 (64-19-7), AcOH
PRO VII, **507274**
YDS 33.0 %
T.KW REFLUX
KW alkylation; N-alkylation
NTE reaction:VI -> VII

L55 ANSWER 8 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199922160 CHEMINFORMRX
TI Quinoxaline Chemistry. Part 12. 3-Carboxy-2[phenoxy]-6(7) Substituted Quinoxalines and N-[4-(6(7) Substituted-3-carboxyquinoxalin-2-yl)hydroxy] Benzoylglutamates. Synthesis and Evaluation of in vitro Anticancer Activity.
AU VITALE, G.; CORONA, P.; LORIGA, M.; PAGLIETTI, G.
CS Ist. Chim. Farm. Tossicol., Univ. Sassari, I-07100 Sassari, Italy
SO Farmaco, 53(8), 594-601 (1998)
CODEN: FRMCE8 ISSN: 0014-827X
LA English
AB Thirty quinoxalines, bearing a substituted phenoxy or hydroxybenzoylglutamate group in position 2, are prepared in order to evaluate the in vitro anticancer activity. Screening reveals that only few derivatives, e.g. (IIIc) and (IIId), exhibit moderate growth inhibition activity on various tumor panel cell lines.

RX(1) OF 9 A + B ===> C

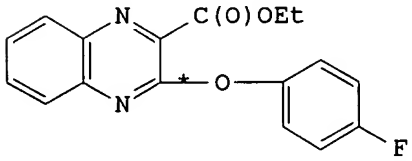


I



II

(1) →

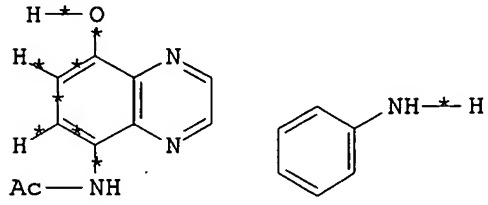


III
YIELD 67.0%

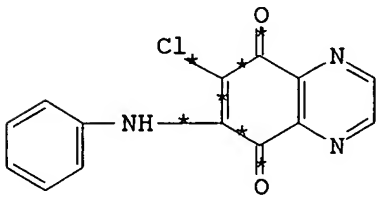
RX(1) RCT I, **200473** (49679-45-0)
II, **12611** (371-41-5)
RGT 1042 (534-17-8), Cs2CO3
SOL 76 (68-12-2), DMF
PRO III, **673122**
YDS 67.0 %
T 70.0 Cel
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III, example: 1

L55 ANSWER 9 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199712148 CHEMINFORMRX
TI A New Synthetic Route to 6,7-Dichloro-5,8-quinoxalinedione and Synthesis of Its Derivatives.
AU HAN, G.; SHIN, K. J.; KIM, D. C.; YOO, K. H.; KIM, D. J.; PARK, S. W.
CS Div. Appl. Sci., Korea Inst. Sci. Technol., Seoul 131-650, S. Korea
SO Heterocycles, 43(11), 2495-2502 (1996)
CODEN: HTCYAM ISSN: 0385-5414
LA English
AB The title compound (IX) is prepared from 4-aminophenol (I) in 8 steps. Key step of the sequence is the chloroxidation of the intermediate sulfate obtained from (VIII). The reaction of (IX) with a variety of nitrogen nucleophiles is investigated.

RX(15) OF 42 COMPOSED OF RX(6), RX(7)
RX(15) M + V ===> W



VIII X



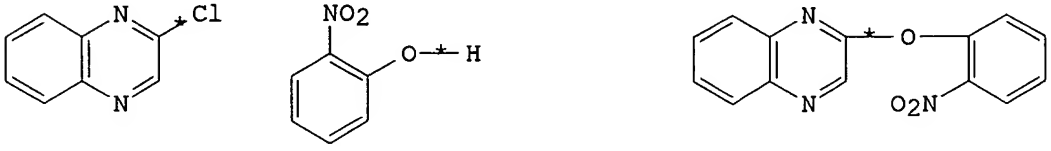
XI
YIELD 81.0%

RX(6) RCT VIII, **520407**
STAGE(1)
RGT 198 (7664-93-9), H2SO4
STAGE(2)
RGT 1338 (7775-09-9), NaClO3
103 (7647-01-0), HCl
T 0.0 Cel
PRO IX, 520408
YDS 63.0 %
KW dearomatisation; halogenation; C-halogenation; chlorination; alkylation
NTE reaction:VIII -> IX
RX(7) RCT IX, 520408
X, **13** (62-53-3)

RGT 318 (7790-86-5), CeCl3
SOL 6 (75-05-8), MeCN
PRO XI, **520409**
YDS 81.0 %
T 25.0 Cel
KW alkylation; N-alkylation
NTE reaction:IX (X) -> XI

L55 ANSWER 10 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199652180 CHEMINFORMRX
TI Synthesis of 2-(2-Nitrophenoxy)quinoxaline and Its Basic Hydrolysis in Aqueous Solutions of Non-Reactive Counter-Ion Surfactants with Bulky Head Groups.
AU CUENCA, A.; STRUBINGER, A.
CS Dep. Quim., Univ. Simon Bolivar, Caracas 1080-A, Venez.
SO Tetrahedron, 52(36), 11665-11672 (1996)
CODEN: TETRAB ISSN: 0040-4020
LA English
AB Micellar effects upon the reaction of hydroxide ions with the title compound (III) are analyzed and the effect of the micellar head group size upon the reaction is investigated. As surfactants cetyltrialkylammonium salts are used. The kinetic data reveal that the basic hydrolysis of (III) to the quinoxalone (IV) can be explained by assuming independent equilibrium distribution for ions in solution between aqueous and micellar pseudophases.

RX(1) OF 1 A + B ===> C



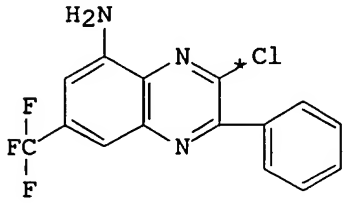
I II III
YIELD 77.0%

RX(1) RCT I, **157891** (1448-87-9)
II, **16226** (88-75-5)
RGT 1160 (1310-58-3), KOH
SOL 76 (68-12-2), DMF
PRO III, **505676**
YDS 77.0 %
T.KW REFLUX
KW arylation; O-arylation; etherification
NTE reaction:I (II) -> III

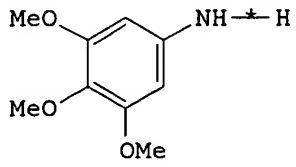
L55 ANSWER 11 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199543192 CHEMINFORMRX
TI Quinoxaline Chemistry. Part 4. 2-(R)-Anilinoquinoxalines as Nonclassical Antifolate Agents. Synthesis, Structure Elucidation and Evaluation of in vitro Anticancer Activity.
AU LORIGA, M.; FIORE, M.; SANNA, P.; PAGLIETTI, G.
CS Ist. Chim. Farm., Univ., I-07100 Sassari, Italy
SO Farmaco, 50(5), 289-301 (1995)
CODEN: FRMCE8 ISSN: 0014-827x
LA English

AB The title compounds, e.g. (VI), act as non-classical antifolic agents with modest to strong anticancer activity. The structure of intermediate (IIIa) is confirmed by an alternative synthesis.

RX(5) OF 12 ...H + K ===> L

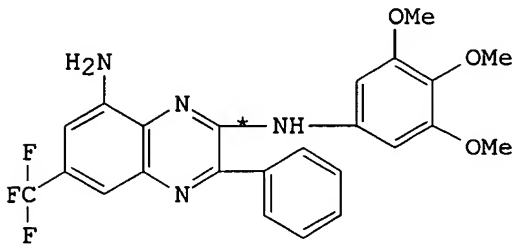


IV



V

(5) →

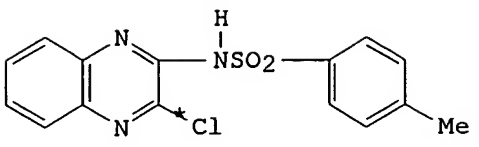


VI
YIELD 69.0%

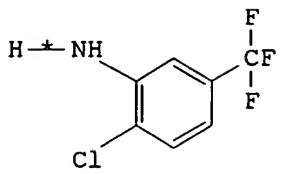
RX(5) RCT IV, **419652**
V, **14704** (24313-88-0)
SOL 182 (71-23-8), PrOH
PRO VI, **419654**
YDS 69.0 %
T.KW REFLUX
KW arylation
NTE reaction:IV (V) -> VI, example: 1
CMT #E0100:(diastereom. mix.)

L55 ANSWER 12 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199512215 CHEMINFORMRX
TI Synthesis, Structure and Chemical Properties of Some N-(3-Chloro-2-quinoxalyl)arylsulfonamides.
AU LITVINENKO, S. V.; SAVITCH, V. I.; BOBROVNIK, L. D.
CS Ukrainskii gos. univ. pishch. tekhnol., Kiev 252017, Ukraine
SO Khim. Geterotsikl. Soedin.(3), 387-392 (1994)
CODEN: KGSSAQ ISSN: 0453-8234
LA Russian
AB The title compounds, which exist as tautomeric mixtures of (III) and (IV), are converted into the derivatives (VI) and (VIII). Reaction of (III)/(IV) with arylamines of type (IX) and (XI) yields the tetracyclic products (X) and (XIII) via intramolecular cyclization.

RX(11) OF 21 ...G + AB ===> AC...

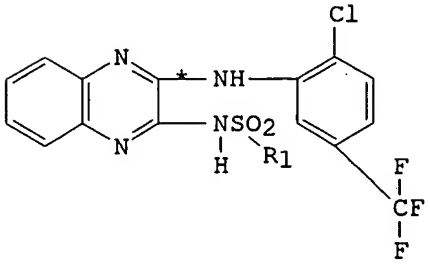


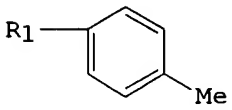
III



XI

(11)





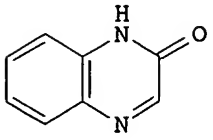
XII
YIELD 83.0%

RX(11) RCT III, **371101**
XI, 18409 (121-50-6)
SOL 76 (68-12-2), DMF
PRO XII, **371111**
YDS 83.0 %
T.KW REFLUX
KW arylation
NTE reaction:IIIb (XI) -> XII

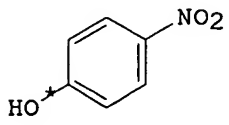
L55 ANSWER 13 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199429215 CHEMINFORMRX
TI Synthesis of 2-(4-Nitrophenoxy)quinoxaline and Its Reactions with the Hydroxide Ion in Micellar Systems.
AU CUENCA, A.; BRUNO, C.; TADDEI, A.
CS Dep. Quim., Univ. Simon Bolivar, Caracas 1080-A, Venez.
SO Tetrahedron, 50(7), 1927-1934 (1994)
CODEN: TETRAB ISSN: 0040-4020
LA English
AB The title compound (III), which is generated from the quinoxalinol (I), reacts with OH- in the presence and absence of micellar systems to afford the ketone (IV). Cationic micelles of cetyltrimethylammonium chloride and bromide and tetradecyltrimethylammonium chloride and bromide speed the reaction. In addition, it is found that the second- order rate constant in

water is higher than constants at the micellar pseudophase.

RX(1) OF 3 A + B ===> C...

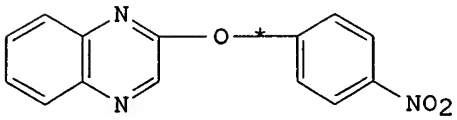


I



II

(1) ⟶

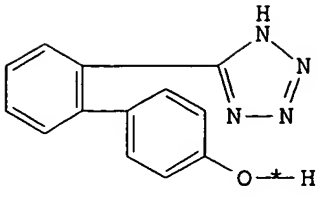


III

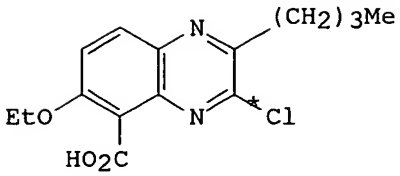
RX(1) RCT I, **323073**
II, **3158** (100-02-7)
STAGE(1)
RGT 181 (10025-87-3), POCl3
461 (10026-13-8), PCl5
STAGE(2)
RGT 1160 (1310-58-3), KOH
YDS 57.0 %
PRO III, **323074**
KW arylation; O-arylation; etherification
NTE reaction:I 2.(II) -> III
CMT Ratio = 3.5:1 for products 1,2

L55 ANSWER 14 OF 14 CHEMINFORMRX COPYRIGHT 2005 FIZ CHEMIE on STN
AN 199352202 CHEMINFORMRX
TI Quinoxaline N-Oxide Containing Potent Angiotensin II Receptor Antagonists: Synthesis, Biological Properties, and Structure-Activity Relationships.
AU KIM, K. S.; QIAN, L.; BIRD, J. E.; DICKINSON, K. E. J.; MORELAND, S.; SCHAEFFER, T. R.; WALDRON, T. L.; DELANEY, C. L.; WELLER, H. N.; MILLER, A. V.
CS Bristol-Myers Squibb Pharm. Res. Inst., Princeton, NJ 08543-4000, USA
SO J. Med. Chem., 36(16), 2335-2342 (1993)
CODEN: JMCMAR ISSN: 0022-2623
LA English
AB A range of potent angiotensin II receptor antagonists containing a quinoxaline residue are prepared. Their efficacy is evaluated by radioligand binding studies using rat adrenal cortical membranes. It is found that analogs having a N-oxide function, e.g. (VI), are more potent antagonists than the parent nonoxidized compounds, e.g. (V).

RX(1) OF 3 A + B ===> C...

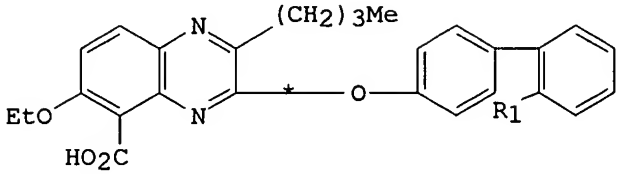


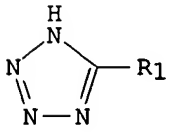
IV



II

(1) →





V
YIELD 84.0%

RX(1) RCT IV, **282214** (150368-30-2)
II, **282213** (150368-44-8)
RGT 1042 (534-17-8), Cs2CO3
SOL 76 (68-12-2), DMF
PRO V, **282215** (150368-48-2)
YDS 84.0 %
T 70.0 Cel
TIM 15 hr
KW arylation; O-arylation; etherification
NTE reaction:IV (II) -> V

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